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GeoPEARL_DE

a Tool for Spatial Modelling of Pesticide Leaching Behaviour in Germany

by

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(Jörg Bangert)

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Abstract

The calculation of predicted environmental concentrations of active ingredients in groundwater is a common procedure in the European authorisation process for plant protection products. By means of the simulated concentrations, the behaviour of a substance can be evaluated and authorisation processes are supported. Since several years, a set of modelling software which is enhanced continuously is used in the evaluation process to fulfil the requirements of the authorities of the European Union. For harmonisation of the model use, standard scenarios of the environment were developed. The European FOCUS groundwater workgroup created a set of nine scenarios for Europe which are implemented in the current modelling software. The practical experience with the usage of these standard scenarios showed some limitations caused by the small range of combinations of environmental parameters within the nine scenarios. For higher tier risk assessments, it is requested to evaluate the substance behaviour on the basis of a wider range of parameter combinations. Furthermore, the attention in the regulatory process turn more and more to the spatial pattern of the environmental parameters such as soil and climate in relation to the area of potential use of a substance. The usage of spatial modelling tools is an approach to fulfil these requirements. In the past, several applications for spatial modelling were set up. One program – GeoPEARL – is based on the PEARL modelling software which is already used in the context of regulatory exposure assessments. It was developed in the Netherlands by the Dutch institutions Alterra Green World Research and the National Institute of Public Health and the Environment (RIVM) and meets the requirements of the Dutch national authorities. The software provides several thousand environmental scenarios which cover the whole range of agricultural conditions in the Netherlands. A single PEARL run can be conducted for each scenario and the results can be presented and analysed using geographic information systems. The GeoPEARL approach is build up in a way that it is possible to transfer it to other regions. Thereby, a new set of scenarios which represents the requested region and a new parameterisation of the software need to be created. It is obvious that this existing application could be used as a tool for advanced spatial modelling for Germany and therefore, there is a need to generate a German set of scenarios. The work presented here follows this intention and describes the generation of a spatial schematisation of Germany which can be used for the parameterisation for the German approach of GeoPEARL – GeoPEARL_DE. The spatial schematisation is generated using spatial data sets of soil, climate, crop statistics and land cover. The soil data were derived from the German soil map BÜK 1000. Daily weather data are available in the MARS database which has a fairly coarse spatial resolution. Therefore, the MARS data were scaled to a higher resolution using a 1 km x 1 km raster data set with long-term values of precipitation and temperature which is provided by the German weather service. Information on the cultivated crops per administrative unit is available within the agricultural census of the Federal Statistical Office of Germany. The CORINE land cover data set is used to derive the data on land use in Germany. The spatial schematisation for GeoPEARL_DE was generated by overlaying the data on land use, soil and climate to get a set of different soil-weather scenarios. The overlay procedure results in 7744 unique combinations. These scenarios were parameterised according to the requirements of the application using the provided soil profiles, the daily weather data and the crop statistical information. Afterwards,

the new parameterisation of GeoPEARL was tested. Regarding the hydrology, it was shown that the amounts of percolated water reaching the groundwater are overestimated because of a non-realistic description of the lateral discharges in the model. With respect to the soil parameters, it is assumed that the organic matter content of the subsoil is too low which has an important influence on the leaching behaviour of the chemicals. Further improvements of the parameterisation are therefore required. New approaches to the simulation of the hydrology have to be implemented in the model itself which need to be conducted by the software developer. The organic matter content in subsoil should be investigated in further studies and then, the humus amounts can be adapted.

GeoPEARL_DE can be used for different purposes. It represents an evaluation tool in the context of a higher tier risk assessment in the regulatory process. Besides this, the application is appropriate to find hot spots of higher leaching risks where advanced monitoring of groundwater can be recommended. Currently, GeoPEARL_DE is used by the BASF AG for the evaluation of spatial pattern of potential leaching risk of substances in Germany. In this context, an abstract of this work was sent to the German authorities in 2006 to present the modelling tool. The results of the GeoPEARL_DE simulations were used to identify regions for groundwater monitoring.

Zusammenfassung

In der EU wird seit längerem für die Beurteilung des potentiellen Eintrags von Pflanzenschutzmitteln in das Grundwasser auf die Berechnung von so genannten Predicted Environmental Concentrations (PEC) zurückgegriffen. Mit Hilfe von Simulationsmodellen können PEC errechnet und das Verhalten einer Substanz beurteilt werden. Die Simulationen sind Grundlage für die Entscheidung über die Zulassung eines Mittels. Seit einigen Jahren wird dabei auf eine Auswahl von Modellen und Anwendungen zurückgegriffen, die ständig nach dem neuesten Stand der Technik weiterentwickelt werden. Um die Anwendung der Modellsoftware zu vereinfachen und zu standardisieren, wurde die Verwendung von vordefinierten Umweltszenarien eingeführt. Die FOCUS Arbeitsgruppe „Grundwasser", die für die EU-Kommission Standards im Bereich Modellierung von Pflanzenschutzmitteln entwickelt, hat dazu neun Szenarien entwickelt, die für Europa gültig sind. Die Anwendung dieser Szenarien hat allerdings gezeigt, dass sie nicht für alle potentiellen Fragestellungen ausreichend sind. Vor allem für höherwertige Risk Assessments wird eine größere Anzahl unterschiedlicher Kombinationen von Umweltparametern und Szenarien benötigt. Hinzu kommt, dass immer öfter die Frage gestellt wird, ob die getesteten Umweltparameter überhaupt im möglichen Anwendungsgebiet einer Substanz vorkommen und die Tests somit überhaupt relevant sind. Die Antworten auf derartige Fragestellungen können durch den Einsatz von Modellen gegeben werden, die das Verhalten von Pflanzenschutzmitteln räumlich modellieren. Dazu wurden in Vergangenheit mehrere Ansätze entwickelt. Einer dieser Ansätze beruht auf der Software PEARL, die schon länger für die Berechnung von Substanzkonzentrationen im Grundwasser genutzt wird. Dieses Werkzeug zur räumlichen Modellierung nennt sich GeoPEARL und wurde in den Niederlanden von Alterra Green World Research und dem Gesundheits- und Umweltministerium (RIVM) entwickelt, um die dortigen Anforderung für die Zulassung von Pflanzenschutzmitteln zu erfüllen. Die Software stellt mehrere tausend Szenarien zur Verfügung, die eine große Bandbreite der Umweltbedingungen in der holländischen Landwirtschaft abdecken. Für jedes Szenario wird mit Hilfe von PEARL die Auswaschung von Substanzen ins Grundwasser simuliert, die dann unter Verwendung von GIS-Werkzeugen präsentiert und analysiert werden kann. GeoPEARL ist so aufgebaut, dass es auch auf andere Regionen übertragen werden kann. Dazu müssen die entsprechenden räumlichen Datensätze zu Szenarien kombiniert werden, die dann die Grundlage für Simulationen bilden. Um für Deutschland eine Applikation zur räumlichen Modellierung des Eintrags von Pflanzenschutzmitteln ins Grundwasser zu entwickeln, wurde der GeoPEARL-Ansatz aus den Niederlanden gewählt. Die Entwicklung von Szenarien für Deutschland, die für GeoPEARL-Berechnungen genutzt werden können, ist Gegenstand der vorliegenden Arbeit. Die deutsche Parametrisierung wird GeoPEARL_DE genannt. Die Szenarien wurden unter Verwendung von Daten zum Boden, Klima, zur Anbaustatistik und zur Landnutzung entwickelt. Die Bodendaten wurden der Bodenübersichtskarte BÜK 1000 entnommen. Tagesgenaue Wetterdaten entstammen der europäischen MARS Datenbank, die allerdings eine recht grobe räumliche Auflösung aufweist. Die MARS Daten konnten aber mit Hilfe von langfristigen Werten des Deutschen Wetterdienstes zur Temperatur und zum Niederschlag, die für ein 1 km x 1 km-Raster vorliegen, auf diese Auflösung skaliert werden. Der deutsche Agrarzensus des Statistischen Bundesamtes stellt die Anbaustatistiken bezogen auf Verwaltungseinheiten zur

Verfügung. Die Informationen zur Landnutzung wurden aus der Landnutzungsinformation der CORINE Datenbank abgeleitet. Die Daten zur Landnutzung, zum Klima und zum Boden wurden in einem Overlay-Verfahren in einem GIS verschnitten. Dabei ergaben sich 7744 Umweltszenarien mit unterschiedlichen Klima- und Bodeneigenschaften. Diese Szenarien wurden anhand der Vorgaben der Software parametrisiert und dann auf Funktionsweise und Plausibilität geprüft. Die Simulation der Hydrologie führt in der bestehenden Parametrisierung zu sehr großen Mengen an Bodenwasser, die das Grundwasser erreichen. Diese Überschätzung der Grundwasserneubildungsrate beruht auf der ungenügenden Simulierung von lateralen Wasserabflüssen im Boden und an der Oberfläche. Eine weitere Betrachtung der Bodenparameter führt zu der Vermutung, dass die Humusgehalte im Unterboden im Allgemeinen zu niedrig angenommen werden. Das hat entscheidenden Einfluss auf das simulierte Verhalten der Pflanzenschutzmittel, da diese an Humuspartikeln adsorbieren können und ihre Auswaschung dadurch vermindert wird. Eine Verbesserung der bestehenden Parametrisierung scheint daher angebracht: Die Simulation der Hydrologie muss innerhalb der Software geändert werden, wogegen der Bodenparameter Humus in der Parametrisierung selbst geändert werden kann. Dazu sollten weitere Untersuchungen zum Humusgehalt im Unterboden anhand tatsächlicher Bodenprofile vorgenommen werden.

GeoPEARL_DE kann für verschiedene Zwecke genutzt werden. Zum einen stellt es ein Hilfsmittel zur Entscheidungsfindung in höherwertigen Risk Assessments im Zulassungsverfahren für Pflanzenschutzmittel dar. Darüber hinaus kann die Applikation dazu genutzt werden, im Untersuchungsgebiet Schwerpunkte für das Risiko von Substanzeinträgen ins Grundwasser zu identifizieren. Dort kann dann gezielt ein Programm zum Grundwassermonitoring gestartet werden.

GeoPEARL_DE wird zurzeit von der BASF AG dazu genutzt, das räumliche Muster von potentiellen Auswaschungsrisiken zu untersuchen. Dazu wurde die Applikation 2006 in einer kurzen Abhandlung den deutschen Behörden vorgestellt. Bei dieser Untersuchung ging es um die Identifizierung von sinnvollen Standorten für Grundwassermonitoring.

Table of Contents

List of Figures

List of Appendix Figures

List of Tables

List of Appendix Tables

List of Equations

List of Abbreviations

AF-model	**A**ttenuation **f**actor model
ASA-CSSA-SSSA	**A**merican **S**ociety of **A**gronomy – **C**rop **S**cience **S**ociety of **A**merica – **S**oil **S**cience **S**ociety of **A**merica
APECOP	**A**ssessing the **P**redicted **E**nvironmental **C**oncentrations **of** **p**esticides
ATKIS	**A**mtliches **T**opographisch-**K**artographisches **I**nformations**s**ystem
BGL	**B**oden**g**roß**l**andschaft (aggregation level of the German soil map)
BGR	**B**undesanstalt für **G**eowissenschaften und **R**ohstoffe (Federal Institute for Geosciences and Natural Resources)
BKG	**B**undesamt für **K**artographie und **G**eodäsie (Federal Agency for Cartography and Geodesy)
BÜK 1000	**B**oden**ü**bersichts**k**arte 1:1,000,000 (Soil Map, scale: 1:1,000,000)
CLC	**C**ORINE **l**and **c**over
CORINE	**Co**o**r**dinated **in**formation on the **e**nvironment
DHDN	**D**eutsches **H**aupt**d**reiecks**n**etz (GCS used in Germany)
DRASTIC	**D**epth of water table, **r**echarge, **a**quifer media, **s**oil media, **t**opography, **i**mpact of the vadose zone, **c**onductivity
DWD	**D**eutscher **W**etter**d**ienst (Germany’s National Meteorological Service)
EEA	**E**uropean **E**nvironment **A**gency
EPA	**E**nvironmental **P**rotection **A**gency
ETC	**E**uropean **T**opic **C**entre
EU	**E**uropean **U**nion
FOCUS	**Fo**rum for the **c**o-ordination of pesticide fate models and their **us**e
FOOTPRINT	**F**unctional **Too**ls for **P**esticide **Ri**sk Assessment and Manageme**nt**
GB	**G**iga**b**yte
GCS	**G**eographical **c**oordinate **s**ystem
geoPERA	**Geo**data in **p**robabilistic **e**xposure and **r**isk **a**ssessments
GIS	**G**eographic **I**nformation **S**ystem
GK	**G**auss-**K**ruger-System
GUI	**G**raphical **u**ser **i**nterface
HAD	**H**ydrologischer **A**tlas von **D**eutschland (Hydrological Atlas of Germany)
ID	**Id**entifier
IVA	**I**ndustrie**v**erband **A**grar (Association of the German agricultural industry)
JRC	**J**oint **R**esearch **C**entre
LBA	**L**eit**b**oden**a**ssoziation (aggregation level of the German soil map)
MARS	**M**onitoring of **A**griculture with **R**emote **S**ensing
MPT	Unique combinations of **M**ARS tile, **p**recipitation and **t**emperature
MPTS	Unique combinations of **M**ARS tile, **p**recipitation, **t**emperature and **s**oil
NL	The **N**ether**l**ands
NLfB	**N**iedersächsiches **L**andesamt **f**ür **B**odenforschung (Institute of soil science of Lower Saxony)
OM	**O**rganic **m**atter
P	**P**recipitation
PEARL	**P**esticide **e**mission **a**ssessment at **r**egional and **l**ocal scales
PEC	**P**redicted **e**nvironmental **c**oncentration
PELMO	**P**esticide **L**eaching **M**odel
PRZM	**P**esticide **R**oot **Z**one **M**odel
PT	Unique combinations of **p**recipitation and **t**emperature
RIVM	**Ri**jksinstituut voor **V**olksgezondheid en **M**ilieu (National Institute of Public Health and the Environment of the Netherlands)
UC	**U**nique **c**ombination
SCI	**S**ociety of **C**hemical **I**ndustry
SPADE	**S**oil **P**rofile **A**nalytical **D**atabase of **E**urope
SWAP	**S**oil **W**ater **A**tmosphere **P**lant model
T	**T**emperature
TETrans	**T**race **E**lement **Trans**port
USDA	**U**nited **S**tates **D**epartment of **A**griculture

1 Introduction

Today, the usage of plant protection products is an important instrument in agriculture and cannot be abandoned with regards to an adequate supply of high quality food for the world population. The amount of applied pesticides has risen in the last century due to the increase of the world population and the expansion of agricultural used land, and adverse side-effects became visible. As reaction to this, the application of plant protection products was controlled and restricted by national authorities to protect fauna, flora, and eco-systems and, therefore, human health. Today, pesticides are subject to a high standard registration procedure and their impact on non-target organisms and environmental compartments is analysed.

In Europe, the basis for pesticide registration is the Plant Protection Products Directive (91/414/EEC) of the European Commission. The aim of the Directive is to harmonise the registration of plant protection products within the European Community. Registration of a substance is only possible when it was shown that its impact on the environment and non-target organisms is negligible and shows no adverse effects. Regarding the environmental compartments soil, water and air, the European Commission recommends to evaluate the behaviour of a substance by calculating predicted environmental concentrations (PEC) for risk assessments. For the harmonisation of the PEC calculations, the European Commission founded the **FO**rum for the **C**o-ordination of pesticide fate models and their **US**e (FOCUS) in 1993 (FOCUS, 2007).

Several workgroups were initiated to attend to the different environmental compartments. First a guideline for the simulation of pesticide leaching into groundwater was provided (FOCUS, 1995); in the following years, guidance for the calculation of PEC in soil and in surface water were added (FOCUS, 1997a, 1997b). In 2000, the FOCUS work group on groundwater scenarios published their recommendations for standardised environmental scenarios (i.e. soil, weather and crop management) for the calculation of the PEC in groundwater (FOCUS, 2000). These FOCUS groundwater scenarios are currently used in the European registration procedures.

The FOCUS groundwater working group is currently in the process of specifying a generic tiered assessment scheme for the evaluation of pesticide leaching to groundwater in Europe. For risk assessments in a higher tier, advanced spatial modelling considering area-wide data is intended to be used. Leaching assessment with high spatial resolution (regional or local scale) is one possibility to deliver regulatory endpoints for the national registration procedures of plant protection products. Existing examples of such tools are set up on the commonly used leaching model PEARL and were developed for the national scale in the Netherlands with GeoPEARL (Tiktak et al., 2003, 2004a) and for the European scale with EuroPEARL (Tiktak et al., 2004b).

2 About this work

Currently, a tool for spatial modelling of the leaching behaviour of a plant protection product is not available for Germany. The work presented here describes the set up of such a spatial modelling tool which is based on the Dutch software tool GeoPEARL. A spatial schematisation for Germany integrating data sets on soil, climate and cropping area was developed to parameterise the modelling software which is named GeoPEARL_DE. Simulations with GeoPEARL_DE were carried out and the results were evaluated and presented.

GeoPEARL_DE should serve as a tool for the evaluation of pesticide leaching on the German national scale with respect to higher tier risk assessments. Apart from this, the tool can be used to identify regions where the probability of leaching of a given substance is the highest (identification of areas of interest), e.g. vulnerable areas where monitoring programs could be carried out. Therefore, the work is addressed to experts in risk assessments for pesticide leaching in Germany to support evaluation procedures in the framework of the registration of plant protection products. The spatial schematisation is set up on existing official data sets. New data sets were not generated or collected for this work.

The results of GeoPEARL_DE need to be evaluated with respect to the scale of the input data. Exact predictions of concentrations in groundwater at a specific place cannot be expected. The results of GeoPEARL_DE should be evaluated by monitoring data in further studies. A broad comparison of the modelling results with measured data will go beyond the scope of this work.

The first part of this document gives background information on modelling of predicted environmental concentrations of pesticides within the European context for the reader. The legal context of pesticide usage, as well as the involved institutions and the decision tree for authorisation of pesticides considering the groundwater, is presented. Then, some spatial modelling approaches are described in general and the model application GeoPEARL in detail.

In chapter 4, the data sets used and their preparation for the application in the context of a German schematisation of GeoPEARL are depicted. Following is the generation and the parameterisation of the spatial schematisation which results in a comprehensive data set that can be used for GeoPEARL simulations for Germany. The new spatial schematisation was tested as described in chapter 9. Differences to the original Dutch approach are outlined, as well as some experiences and limitations of the German approach. The results are discussed in the context of their possible fields of application and the constraints of the usability. Finally, perspectives for further applications and developments are given.

3 State of the art in spatial modelling in the EU

3.1 Modelling of PEC groundwater in the EU

3.1.1 Set-up of a first guidance

The basis for pesticide registration in the European Union is the Plant Protection Products Directive (91/414/EEC) of the European Commission that was created by the Council of Ministers in 1991 and came into force in 1993. The aim of the Directive is to harmonise the rules for the registration of pesticides in all member states. This was necessary because differing rules had prohibited the free trade of plant protection products within the European Community. For harmonisation, the Directive ascertains that an active ingredient of a plant protection product has to be listed on a positive list (Annex I of the Directive) before the respective product can be authorised for use in the member states. For the inclusion in Annex I, the producer of the plant protection product has to prepare a dossier for the substance. The dossier is submitted to at least one Member State that is then responsible for the evaluation of the product. The dossier consists of a comprehensive list of all data that are necessary to evaluate the properties of the substance. The data for the active ingredient and at least one product containing this active ingredient must be submitted. The responsible member state evaluates the dossier data, reports them to the European authorities and gives recommendations. After positive evaluation, the active ingredient can be listed in Annex I and a plant protection product including this active ingredient can be authorised for use by the Member States. This approach implies, that in the end of the process, each Member State decides for itself if a plant protection product is authorised for use in its own country.

In the Directive, a uniform evaluation procedure for inclusion in Annex I is recommended. For the harmonisation regarding evaluation of pesticide behaviour in the environment, the European Commission founded the **FO**rum for the **C**o-ordination of pesticide fate models and their **US**e (FOCUS) in 1993. Experts from industry, from the regulatory authorities and from research institutes share in the forum. Several workgroups were initiated to attend to the different environmental compartments as shown in Figure 1.

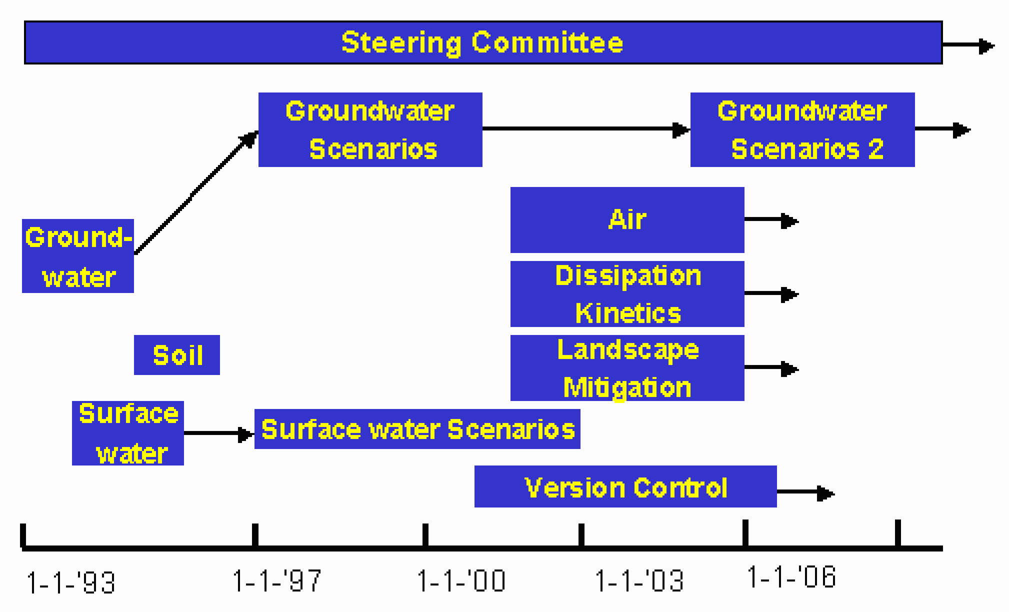


Figure 1: FOCUS workgroups and current status (FOCUS, 2007)

In 1995, the FOCUS groundwater workgroup published the first European guidance for the simulation of pesticide behaviour in the context of the Plant Protection Products Directive (FOCUS, 1995). The aim of the report was to develop a framework for the simulation of pesticide leaching within the EU. The main part of the report deals with the existing modelling software. Features, input parameters, model types and their "philosophy" were described, as well as their limitations and existing validation studies. The software was evaluated to determine if it is appropriate for usage with respect to the FOCUS context. Furthermore, a codex for correct model use was defined in the sense of a "Good Modelling Practice" and a first proposal for a step-wise approach in groundwater risk assessments was given as shown in Figure 2. By means of such a step-wise or tiered approach, the pesticide behaviour is evaluated using different environmental parameters starting with extreme worst-case but simple scenarios and going on with more and more realistic and detailed scenario descriptions. The results of each modelling step are evaluated and if a safe usage of the substance is indicated, no further work is required. Thus, usage can be defined as safe in an early step with simple conditions for non-critical substances to reduce costs and time in the modelling process.

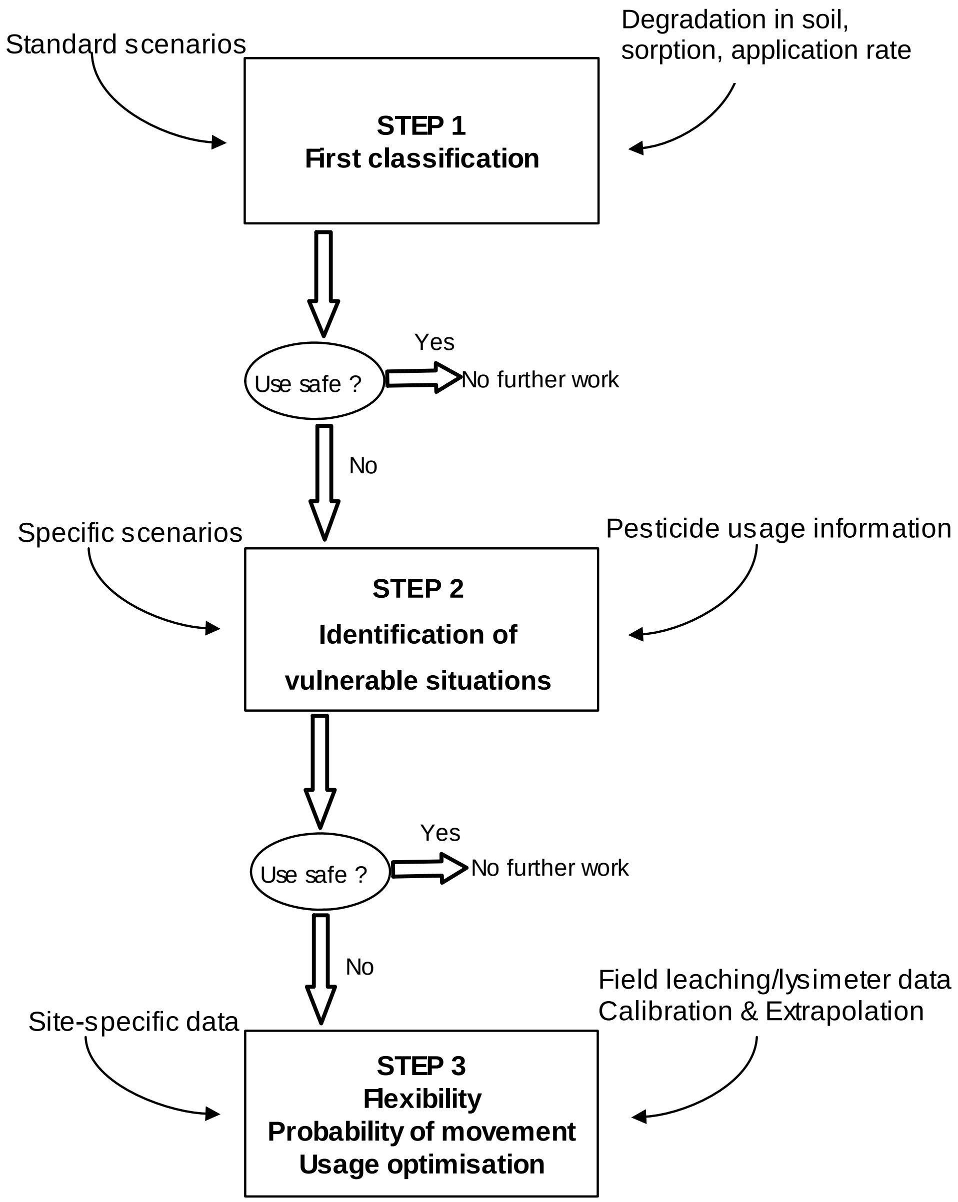


Figure 2: Tiered approach for PEC calculations in the groundwater according to FOCUS (1995)

Step 1 of the tiered approach proposed by FOCUS (1995) describes the standard usage of the existing models with one or more worst-case scenarios, i.e. defined environmental parameters for weather and soil. If the results of this modelling step are below a defined trigger value, the usage of the plant protection product is considered to be safe. If the results do not indicate a safe use, more sophisticated simulations on a higher step will be carried out with respect to information on pesticide usage, site-specific data or existing monitoring studies. This includes the refinement of existing environmental scenarios in order to focus on the intended use-area of a substance, e.g. usage in a crop that does not grow in sandy soils. In this context, spatial modelling and the usage of Geographic Information Systems (GIS) as a useful tool in higher tier risk assessments was not yet mentioned. Nevertheless, the variability of climate and soil in Europe was depicted and the necessity of different environmental scenarios representing different European regions was confirmed. This implies the usage of GIS which can be used to define climate and soil scenarios using overlay procedures.

In the FOCUS guidance document (FOCUS, 1995), an overview of existing scenarios for the simulations was arranged. It was shown that in 1995 only scenarios for the Netherlands and for Germany were defined and used in regulatory risk assessments. With regard to the standardisation of pesticide registration, the workgroup gave a first proposal for pan-European leaching scenarios that could be used in the risk assessments. Ten climatic zones in combination with five soil scenarios were suggested using climate and soil maps of Europe as basis for the proposal. Nevertheless, the proposed scenarios were not yet fully developed because important data, such as daily weather data or comprehensive data on soil profiles were not available. Thus, the suggested scenarios were neither implemented into the modelling software nor into the registration procedure. However, with this report, the working group created the basis for future development of standardised scenarios by recommending environmental parameters that are required for model input.

3.1.2 Development of standard scenarios for leaching risk assessments

After a proposal for standard scenarios in the EU registration procedure and the recommendation for their development by FOCUS (1995), the FOCUS workgroup on groundwater scenarios started its work in 1997. The aim of the workgroup was to develop comprehensive standard scenarios as well as to implement them into the current modelling software. With the help of standardised modelling procedures, FOCUS wanted to fulfil the following goals (see FOCUS, 2000):

- Risk assessments are standardised to increase the consistency within the EU.
- Speed and simplicity of the usage of simulation models will increase because less user inputs are required and the software shells will be optimised for the user.
- The usage of the standard scenarios is defined to give guidance on further registration of plant protection products for Annex I of the Directive of the European Commission.
- Using standard scenarios will decrease the influence of the user. The transparency of the model calculations will increase and simultaneously the acceptance by registrants and authorities.

The final report with the results of the workgroup was published in 2000 (FOCUS, 2000). Nine standard scenarios were developed. They describe the majority of agricultural used land in the EU member states (at this time: EU-15). Special environmental conditions, as well as crops that are only grown in small regions are not considered. The location of the scenarios and their characteristics are given in Figure 3 and Table 1.

Figure 3: **Locations of the nine FOCUS groundwater scenarios (FOCUS, 2000)**

Table 1: **Characteristics of the nine weather and soil scenarios created by FOCUS (2000)**

Location	Soil type (USDA[1])	Organic matter (OM) [%]	Annual average air temperature [°C]	Annual sum of precipitation [mm]
Châteaudun	silty clay loam	2.4	11.3	648+ I*
Hamburg	sandy loam	2.6	9.0	786
Jokioinen	loamy sand	7.0	4.1	638
Kremsmünster	loam/silty loam	3.6	8.6	900
Okehampton	loam	3.8	10.2	1038
Piacenza	loam	1.7	13.2	857 + I*
Porto	loam	6.6	14.8	1150
Sevilla	silty loam	1.6	17.9	493 + I*
Thiva	loam	1.3	16.2	500 + I*

[1] soil classification according to United States Department of Agriculture (USDA) *irrigation

The names of the scenarios were derived from the respective weather station. Nevertheless, the scenarios do not represent specific fields and they do not reflect the conditions of agriculture in the EU member state where they are located. The set of the scenarios as a whole can be considered as representative for the main part of the agricultural used land in the EU.

The development of the scenarios by the FOCUS workgroup led not only to recommendations of usable scenarios but to their implementation in the current modelling software that is used in regulatory context for groundwater risk assessments. In the first FOCUS groundwater report (FOCUS, 1995), a set of models was presented that was used for the evaluation of leaching behaviour. FOCUS (2000) reduced the number of models to four software packages which include the parameterisation of the nine standard scenarios. Table 2 gives an overview of the models.

Table 2: Overview of leaching models recommended by FOCUS (derived from FOCUS, 1995, 2000 and 2007)

Name	Developers	Reference	Intended model use
PELMO (PEsticide Leaching MOdel)	M. Klein Frauenhofer Institut für Umweltchemie, Schmallenberg, Germany,	Klein (1995)	The model predicts leaching of a substance in soil under consideration of runoff and erosion.
MACRO	N. Jarvis, Swedish University of Agricultural Science (SLU, Uppsala)	Jarvis (1994)	The model simulates pesticide movement in the soil under consideration of preferential flow in macropores. Only the Châteaudun scenario is implemented.
PEARL (Pesticide Emission Assessment at Regional and Local scales)	A. Tiktak, D. v. Kraalingen, E. v. d. Berg, J. Boesten, M. Leistra, T. v. d. Linden, RIVM and Alterra (NL)	Tiktak et al. (2000)	The model predicts leaching of a substance in soil.
PRZM (Pesticide Root Zone Model)	R.F. Carsel et al., EPA USA	Carsel et al. (1998)	The model calculates the substance movement in surface and subsoil as well as volatility, runoff and erosion.

The FOCUS versions of the models PELMO, PEARL, PRZM and MACRO (only Châteaudun scenario) are distributed with the implemented FOCUS scenarios. Only these versions are authorised to be used in the regulatory process. They are available on the homepage of FOCUS (http://viso.jrc.it/focus/index.html, 2007-03-17) for free usage in the context of plant protection authorisation.

The FOCUS standard scenarios include the following information:

- Daily weather data with
  - Temperature (daily minimum and maximum)
  - Precipitation
  - Global radiation
  - Average vapour pressure
  - Average wind speed
  - Reference evapotranspiration
- Soil data with
  - Thickness of horizons
  - Soil texture
  - Organic matter content
  - pH-value
  - Bulk density
  - Soil hydraulic parameters
- Crop parameters with
  - Critical pressure heads for water uptake
  - Root density
  - Development stages
- Crop management parameters with
  - Emergence dates
  - Harvest dates
  - Irrigation

The scenarios were defined with the intention to reflect the majority of agricultural used land in the EU. Therefore, appropriate climate stations and soil profiles were selected. The scenarios should also describe an overall vulnerability for leaching which represents the 90th percentile of all possible situations. The FOCUS work group decided to select soil profiles as well as climate stations which show each an 80th percentile of vulnerability to match the criterion of an overall 90th percentile if they are combined. The 80th percentile for the climate is derived by calculating the substance leaching for a period of 20 years. The 80th percentile of the resulting 20 leaching concentrations is then taken as the final result. For the soil profiles, the 80th percentile was defined by expert judgment (see FOCUS, 2000).

For the selection of the climate stations, the area covered by the EU member states was divided into climate regions considering the annual sum of precipitation and the annual mean temperature. The nine climate regions with the highest ratio of arable land were chosen and appropriate weather stations were selected (Table 3). The names of the scenarios were derived from the names of the respective weather stations. The scenarios are distributed throughout Europe and cover a broad range of climatic conditions in Europe (see Figure 3). For each climate station, daily weather data for a time series of 20 years were selected to match the 80th percentile criterion. In the case of substance application every two or three years, the FOCUS standard scenarios provide time series of 40 and 60 years which were derived by duplicating and triplicating the existing 20 weather years.

Table 3: Arable agriculture in EU climate zones (FOCUS, 2000)

Annual sum of precipitation [mm]	Annual average 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 soil profiles were selected by expert judgment. They should represent the range of soil conditions in the EU with respect to the weather conditions to avoid unrealistic weather-soil scenarios. The soil parameters should be significantly more vulnerable than an ”average” soil in the respective agricultural area, i.e. in general they should have less organic matter content and a higher portion of sand which leads to higher pesticide leaching.

As crop parameters and crop management parameters change in relation to the climatic and soil conditions, appropriate parameters were selected for each scenario. They were derived by judgment of local experts. Furthermore, for each scenario, crops were selected that are grown under the respective environmental conditions in the agricultural area. The relation between scenario and crop is fixed in a standard risk assessment and thus a realistic combinations can always be confirmed. If a crop is not relevant for a certain scenario, no crop parameters and no data on crop management were defined and no calculations for the respective crop are possible for this scenario.

With the FOCUS report on groundwater scenarios (FOCUS, 2000), the usage of the four described models and the nine groundwater scenarios is obligatory for the inclusion of active ingredients in Annex I of the Council Directive (see chapter 3.1.1). For the inclusion, the simulated concentration of a substance must be less then a trigger value. The trigger value is currently defined at 0.1 µg L^{-1} at an evaluation depth of 1 m. The simulated concentration is derived as follows: Leaching behaviour of a substance is simulated for a time period of 20 years in all FOCUS scenarios. For each year, an average substance concentration based on daily values at a soil depth of 1 m is calculated. The 80th percentile of the resulting 20 concentration values is taken for evaluation. In the case of substance application every two or every three years, the average of the two or three years between each application was calculated, which results again in 20 concentration values. With respect to the selected soil profiles which represents the 80th percentile of vulnerability for soils, this value represents the overall 90th percentile for leaching vulnerability in Europe. The active ingredient can be included in Annex I if the trigger value is not exceeded in at least one of the defined scenarios.

As described in chapter 3.1.1 the usage of a plant protection product in its own country has to be authorised by each Member States. The authorisation has to be conducted with respect to the modelling results of Annex I inclusion. If specific crop scenarios exist within one Member State which are not covered by the standard scenarios (e.g. hop in Germany), further modelling considering the specific field conditions can be required by the national authorities if the usage in such crops is requested. The standard scenarios where the calculated concentration exceeds the trigger value can be used for the identification of critical usage scenarios. For those scenarios, more sophisticated evaluation methods such as field studies need to be carried out to show safe use.

For the authorisation of plant protection products in the Member States, it is recommended that the national authorities use the proposed modelling software and the groundwater scenarios for the evaluation of the leaching behaviour. Nevertheless, several Member State prefer their own approach, e.g. Germany which proposes the usage of the software tool PELMO 3.0 with a specific German scenario including two different Hamburg weather scenarios and a soil profile located near Borstel, Germany (Michalski et al., 2004).

3.1.3 Development of a decision scheme in leaching risk assessments

For the authorisation procedure according to the Plant Protection Products Directive, only step 1 of the decision scheme described in chapter 3.1.1 and Figure 2 has yet been defined, i.e. the standard FOCUS groundwater scenarios. For the optimisation of the evaluation of pesticide leaching, a fully described tiered approach is required to give a more exact guidance for risk assessment. Furthermore, Tiktak et al. (2000, 2004b) challenged the suitability of a small range of standard scenarios for the evaluation of leaching behaviour. They compared the results of a spatial modelling approach (GeoPEARL, see chapter 3.3) with the results of the Dutch standard scenario for four pesticides. It was shown that the standard scenario supports the registration for two pesticides whereas the results of GeoPEARL lead to a contrary decision. The authors concluded therefore that the number of considered scenarios should be increased to cover a wider range of scenarios and they recommend using advanced spatial modelling in the registration procedure. A spatial modelling approach would consider the variability of the soil, climate and crop parameters in the investigated region. The resulting maps showing the leaching potential would support further evaluation procedures.

In 2003, a new FOCUS groundwater workgroup started its work to refine the tiered approach for a decision scheme in leaching risk assessments (Azimonti, 2006; see Figure 1). A proposal for the decision scheme is given in Figure 4.

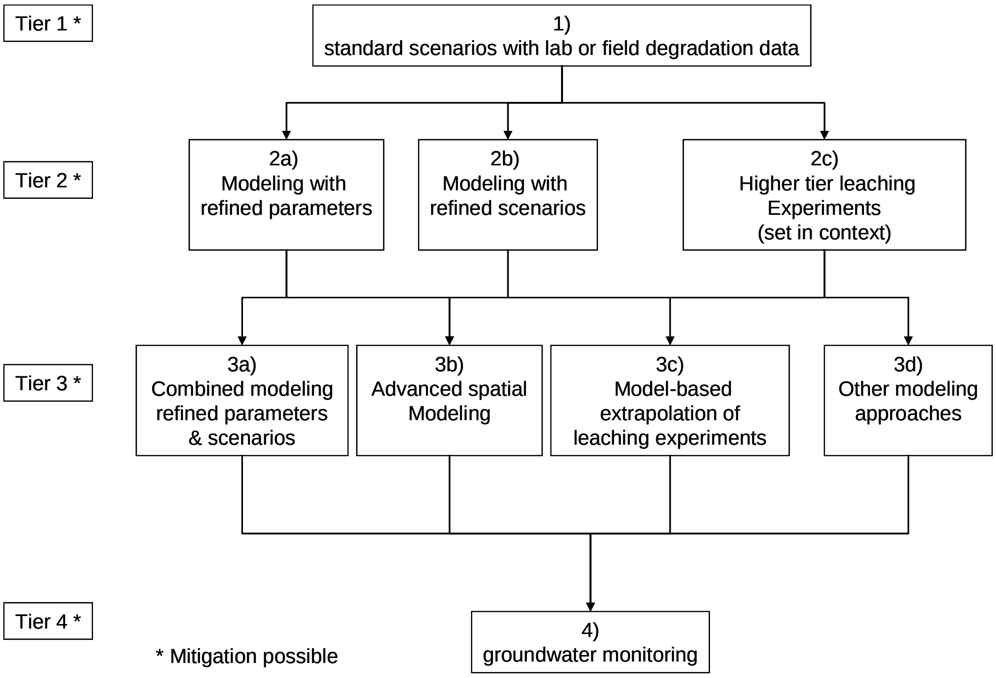


Figure 4: FOCUS proposal for generic tiered assessment scheme for groundwater (Azimonti, 2006)

Step 1 of the tiered approach includes the described PEC calculations using the FOCUS standard scenarios which are simple and rapid to use but lead to conservative simulation results. The higher tiers will represent more realistic and specific approaches to the proposed use pattern of the plant protection product with respect to substance parameters and refined scenarios. Therefore, it can be shown that the use of the substance is safe within the limits of the intended cropping scenario. Otherwise, non-critical substances can be identified on a lower level of simulations and time need and costs can be reduced. In Tier 3 of the proposed decision scheme, advanced spatial modelling using area-wide data is recommended. The intention is to simulate the leaching behaviour under consideration of the existing combination of environmental parameters (climate and soil) within the actual cropping area. Therefore, extreme weather-soil combinations that are not relevant for the respective crop will be excluded from the calculations and the results are more realistic. With the recommendation of the usage of advanced spatial modelling, the usage of GIS is intended to become an optional tool in the regulatory process for plant protection products.

3.2 Approaches to spatial modelling

The combination of GIS and model software and the application of spatial modelling to improve the risk assessments of non-point source pollutants have been introduced by different authors for a long time. Corwin et al. (1996) depicted in their overview of the ASA-CSSA-SSSA Bouyoucos Conference held in 1995 in California that in years past, the focal point of the investigation of chemicals in the environment moved from point source pollutants to non-point source pollutants, such as salts, agro-chemicals or heavy metals. The consideration of such diffuse pollutants is much more sophisticated because their impact is not limited to a specific region and, in most cases, the relation of cause and effect is not obvious because of their low concentration. The ubiquity and the chronic effects of the non-point source pollutants will need improved investigation strategies and risk assessments of such chemicals, particularly the agro-chemicals because they are used in wide-spread areas.

It is recommended to use spatial modelling approaches for the evaluation because the behaviour of diffuse distributed chemicals depends on environmental parameters which vary in space and the different combination of parameters has to be considered in the investigations. As GIS are specialised for the management of spatial data, they are first choice in risk assessments. With the implementation of a GIS in the modelling procedure, it is possible to manage the large amount of spatial data, to combine the different parameters required for model input and to provide the set of input data for the modelling software. Furthermore, GIS can be used for the evaluation and presentation of the model results.

The authors propose an abstract structure for a spatial modelling tool. It should be composed of a model that describes the substance transport in the soil, the input data for the model which are spatially distributed and the GIS which manages the data. Up to the time of the conference, no software package was available that integrates GIS and modelling software in one product. Therefore, the two systems - GIS and model software - are coupled to get a spatial modelling tool. Different levels of such coupling are possible: In a low level, the GIS can be used for data preparation and the presentation of the results. The two systems still remain separated and the user manages the data exchange. In a high level, the two systems revert to the same database and data exchange is managed by the software. In the article, a lot of references are listed that show that the usage of GIS in the modelling context is broadly accepted. As a conclusion, the authors look upon the application of GIS in the modelling context as an appropriate approach to more sophisticated evaluation of non-point source pollutants. They remarked that for the interpretation of the modelling results, the scale and the accuracy of the input data is very important because a GIS can lead to the illusion of high accuracy that is not reflected by the input data.

Some examples for spatial modelling tools are given by Petach et al. (1991), Vaughan et al. (1994) and Lobo-Ferreira et al. (1997). The tool GeoPEARL which is subject of this work is described in chapter 3.3. The study of Petach et al. (1991) intends to give recommendations for field management with respect to the risk of pesticide leaching. The water flux and pesticide movement is simulated with a one-dimensional convection-dispersion-based solute transport model. The soil and weather data from a trial site in Albany, New York are used to evaluate the spatial variability of pesticide leaching for a time-series of 25 years.

Vaughan et al. (1994) expand the existing one-dimensional model TETrans to TETransgeo by implementing a GIS-module. TETransgeo represents a low level coupling of model and GIS in the sense of Corwin et al. (1996). The model, which simulates the water and the solute fluxes in the unsaturated zone of a soil profile, runs independently of the GIS. With the help of the GIS, a set of locations can be prepared which includes all necessary input data for the model. For each location, one model run is carried out and the results can be evaluated and presented with the help of the GIS. The intention of the model is to optimise irrigation strategies in agriculturally used land to avoid negative side-effects, e.g. salinisation.

Lobo-Ferreira et al. (1997) developed a map of groundwater vulnerability in Portugal using the DRASTIC index. The focus is not on pesticide vulnerability but on pollutants in general, e.g. nutrients, heavy metals and pathogens. GIS were used to combine the input parameters and to calculate the index.
The index is derived from the following input parameters:

- **D**epth of water table
- Groundwater **R**echarge
- **A**quifer material
- **S**oil type
- **T**opography
- **I**mpact of vadose zone
- Hydraulic **C**onductivity

The work does not represent modelling in the sense of predicting environmental concentrations but it shows that GIS are useful for the realisation of environmental risk assessments.

Current approaches to spatial modelling were outlined by different authors in poster sessions or oral presentations during workshops and conferences in the last years. The next section describes some of the present thoughts.

At the third European Modelling Workshop held in Catania, Italy, in 2004, Klein (2004) described a concept for a higher tier GIS study in the framework of the FOCUS groundwater scenarios based on the existing FOCUS model PELMO. The author used different European data sets for the evaluation of the existing nine standard scenarios. Furthermore, the performed GIS study gives an impression of the usability of spatial modelling tools in the regulatory context. Further tools that were developed in the FOCUS context are GeoPEARL (Tiktak et al., 2002, 2003) and EuroPEARL (Tiktak et al., 2004b). An overview of the PEARL model family is given in chapter 3.3.

Hollis et al. (2006) presented an advanced spatial modelling approach for the European level at the SCI conference on Pesticide Behaviour in Soils, Water and Air in Warwick, UK. They used pan-

European data sets such as the climate database MARS (**M**onitoring of **A**griculture with **R**emote **S**ensing) and the Soil Geographic Database for Europe which were combined to derive a set of relevant climate-soil scenarios. These scenarios were parameterised and simulation runs with stochastic modelling programs were carried out. The result is a probability distribution of predicted environmental concentrations that can be used for decision support in higher tier assessments.

Leterme et al. (2006) show the differences in simulation results if calculations were carried out based on interpolated spatial data or if the model calculations were based on point data and interpolated to the space. The authors used two different models for the investigation – a linear model AF (Attenuation Factor) and a non-linear model GeoPEARL. The results show differences between the two models and between the two modelling approaches (“interpolating or calculating first”). The study recommends the inclusion of simulations based on point data of environmental properties without spatial interpolation in the assessment to become independent from the interpolation method.

Schad (2006) presented the geoPERA project of the German IVA (**I**ndustrie**v**erband **A**grar) which will give recommendations to the use of **geo**data in **p**robabilistic **e**xposure and **r**isk **a**ssessments. It is proposed to prepare a range of spatial data sets which can be used on different scales – national, regional and local – for the exposure assessment. The spatial data sets should give information about the landscape, e.g. the location of water bodies, of fields and of landscape elements which can involve mitigation of a substance, e.g. planted buffer strips. The data sets that are considered to be appropriate for use range from small to large scale: CORINE land use data, MARS weather data, the German ATKIS data, satellite and aerial images as well as field observations.

The project “FOOTPRINT” (**F**unctional **Too**ls for **P**esticide **Ri**sk Assessment and Manageme**nt** (Dubus, 2006) which was founded by the EU within the 6th framework program will give further ideas on the improvements in pesticide risk assessment. The aim of the initiative is to develop a set of spatial modelling tools for different spatial scales. With the help of the tools, decision makers on different levels (farmers, water managers, policy makers and registration authorities) should be enabled to evaluate the risk of pesticides and to manage their use. The applications are developed on the basis of the current state-of-the-art of pesticide risk assessments and, therefore, a review of the present approaches was carried out (see also www.eu-footprint.org (2007-03-17), Azimonti, 2006; Dubus et al., 2006; Barriuso et al., 2006; Jarvis et al., 2006; Reichenberger et al., 2006).

3.3 The GeoPEARL approach

Tiktak et al. (2002, 2003, 2004a) developed a tool for advanced spatial modelling - GeoPEARL - which is used in the registration process in the Netherlands. The application is based on the modelling software PEARL which is already used in the context of regulatory exposure assessment. The description of the pesticide leaching behaviour that is implemented in PEARL was considered to be appropriate for use because all relevant processes are described within the model. In the next section, an overview of the concepts of PEARL is given and then, the GeoPEARL approach is described in detail.

3.3.1 The basic model – PEARL

The model package PEARL, which is an acronym for **P**esticide **E**mission **A**ssessment at **R**egional and **L**ocal scales, is a one-dimensional, dynamic multi-layer model which simulates pesticide fate in a soil-plant system. The software was developed in 2000 by the Dutch institutions Alterra Green World Research and the National Institute of Public Health and the Environment (RIVM). The current version PEARL 3.3.3 is used in the Dutch and European approach for pesticide registration. A detailed description of the model is given in Leistra et al. (2001) and Tiktak et al. (2000) which are the basis of the following descriptions. Additional information can be found at the PEARL website http://www.pearl.pesticidemodels.eu (2007-03-17).

A one-dimensional model simulates water and pesticide fluxes only in the top-bottom direction and vice versa. Lateral discharges are considered as sink terms. In PEARL, it is assumed that the chemical and physical properties of the soil are uniform within one soil horizon. Thus, no preferential water flow (e.g. in macropores) is simulated. Furthermore, runoff discharge is only calculated if the depth of ponding water at the soil surface exceeds a defined trigger value. As it is assumed in the model that the daily precipitation amounts are evenly distributed through 24 hours, the runoff amounts are significantly underestimated. PEARL simulates the fate of a substance in the soil-plant systems but it does not describe hydrology and soil temperatures. These processes are simulated by the model SWAP (**S**oil **W**ater **A**tmosphere **P**lant model, Van Dam et al., 1997; Kroes et al., 1999). SWAP is embedded in the PEARL model and provides the information on hydrology. PEARL manages the input and output of SWAP so that the user needs only to handle PEARL.

3.3.1.1 Processes in PEARL

The model application simulates a set of processes which have impact on the fate of pesticides in the soil-plant system. In Figure 5, the considered processes are illustrated. PEARL can handle a wide range of chemical substances with different properties because of the comprehensive set of processes that are included in the software.

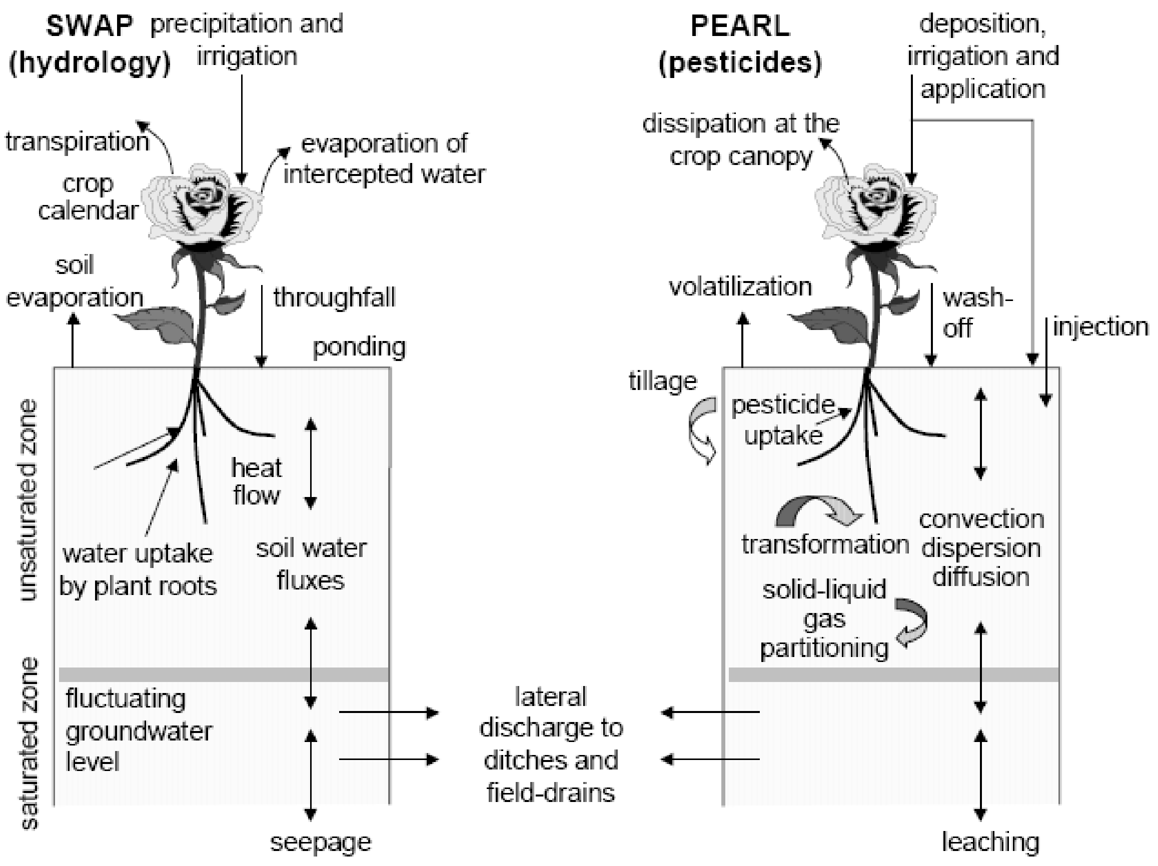


Figure 5: Overview of the processes in the PEARL model (Tiktak et al., 2000)

Processes described by the SWAP model:

- Soil water flow:
  The soil water flow is described with help of the Richards equation which describes the movement of a liquid in a porous system such as the soil. The equation requires parameters of the hydraulic properties of the soil which can be derived from tabulated data or analytical functions as provided by Mualem and van Genuchten (see Tiktak et al., 2000). For PEARL and GeoPEARL, the Mualem-van Genuchten parameters are used for the description of the soil water flow.
- Potential evaporation:
  If no daily values for the potential evaporation are available, SWAP calculates the item using air temperature, solar radiation, wind speed and air humidity.
- Interception of water by the crop canopy
- Water uptake by plant roots:
  Water and solute which is taken up by plant roots cannot reach the groundwater.
- Evaporation of water from soil surface

- Lower boundary condition:
  The lower boundary condition describes the situation at the bottom of the simulated soil column. The behaviour of the seepage fluxes is described. As one option, the level of the groundwater table can be defined.
- Lateral discharge of water:
  With the lateral discharge, the model simulates water discharge by drains or field-ditches.
- Heat flow in soil:
  The soil temperature is important for the degradation of a substance.

Processes described by the PEARL model:

- Pesticide application:
  The pesticide can be applied
    - by spraying the substance to the soil surface
    - by spraying the substance to the crop canopy
    - by incorporation or injection of the substance into the topsoil.

  The effective substance dosage which reaches the soil depends on the factors
    - Interception and dissipation of substance on the crop canopy
    - Drift of sprayed substance from the target field
    - Volatilisation at the soil surface
    - Photochemical transformation.

  PEARL simulates the described processes to calculate the effective substance dosage which is the initial soil dosage for the simulations of the leaching behaviour.
- Convective and dispersive transport of pesticide in the liquid phase of the soil system
- Diffusion of pesticide through the gas and liquid phase of the soil
- Sorption:
  Chemical substances such as pesticides can adhere to particles in the soil, particularly to the organic fraction. Thereby, leaching can be retarded. The sorption behaviour of the substance is therefore an important property.
- Transformation kinetics:
  Pesticides are subject of transformation processes in the soil. The resulting metabolites are considered in the simulation runs. Therefore, appropriate transformation data and the properties of the relevant metabolites have to be specified.
- Pesticide uptake by plant roots:
  The pesticide uptake by plant roots depends on the water uptake simulated by SWAP.
- Lateral discharge of pesticide:
  The lateral discharge of pesticides is proportional to the water discharge simulated by SWAP.

3.3.1.2 Required parameters in PEARL

PEARL requires the following information on environment, substance, crop and crop management as input parameters. Internal model factors which are not spatially distributed are not described here.

Emphasis is given on those parameters which are required in the context of the GeoPEARL parameterisation, i.e. spatially distributed parameters.

Scenario definition:

Soil:

- Soil horizon number
- Horizon thickness (m)
- Sand fraction (kg kg^{-1}) as part of mineral soil
- Silt fraction (kg kg^{-1}) as part of mineral soil
- Clay fraction (kg kg^{-1}) as part of mineral soil
- Organic matter content (kg kg^{-1})
- Bulk density (kg m^{-3})
- pH (required for calculations of pH-dependent substances)
- Parameters describing soil hydraulic properties according to van Genuchten (see Van Dam et al., 1997)
    - Saturated soil water content (m^3 m^{-3})
    - Residual water content (m^3 m^{-3})
    - Parameter alpha (dry) (cm^{-1})
    - Parameter alpha (wet) (cm^{-1})
    - Parameter N (-)
    - Saturated hydraulic conductivity (m d^{-1})
    - Physical saturated hydraulic conductivity (m d^{-1})
    - Parameter L (-)
- Lower boundary condition

Climate:

- Solar radiation, daily values (kJ m^{-2})
- Minimum daily air temperature (°C)
- Maximum daily air temperature (°C)
- Air humidity, daily values (kPa)
- Wind speed, daily values (m s^{-1})
- Precipitation, daily values (mm)
- Reference evapotranspiration, daily values (mm)
- Daily irrigation amounts (mm), optional

Crop:

- Development stage
- Leaf area index (m^2 m^{-2})
- Crop factor for evaporation
- Rooting depth (m)
- Crop height (m)
- Root density
- Parameters of the crop water use
- Interception coefficient

Crop management:

- Application parameters:
    - Application date
    - Application type (e.g. on crop canopy, on bare soil)
    - Dosage of substance (kg ha^{-1})
- Crop calendar:
    - Emergence date
    - Harvest date

Substance definition:

- Molar mass (g mol^{-1})
- Saturated vapour pressure at reference temperature (Pa)
- Solubility in water at reference temperature (mg L^{-1})
- Half-life of substance in soil at reference temperature (d)
- Half-life of substance at crop canopy at reference temperature (d)
- Sorption parameters:
    - Coefficient for sorption on organic matter (K_{om}) (L kg^{-1})
    - Freundlich sorption coefficient (-)
- Diffusion coefficient (m^2 d^{-1})
- Wash-off factor from crop canopy (m^{-1})
- Factor for uptake by plant roots (-)

3.3.2 Description of GeoPEARL

3.3.2.1 Objectives of GeoPEARL

The software GeoPEARL is a spatial modelling tool that was set up in the Netherlands by the same team which had developed PEARL (Tiktak et al., 2002, 2003). The purpose of the new approach was to improve the decision support for pesticide registration in the Netherlands because the existing approach was considered no longer to be suitable: Registration was based on the assessment of one standard scenario which was created by expert judgment. It should represent the 80th percentile of vulnerability regarding the whole range of existing locations. Tiktak et al. (2002) showed that the standard scenario does not fulfil these assumptions for all tested substances. The authors recommended a larger set of scenarios or – more preferred – the introduction of spatial modelling in the registration procedure. As the latter approach was intended to be used by the Dutch authorities, an appropriate software tool was required. Therefore, GeoPEARL, which is based on the modelling software PEARL that is already used in the context of regulatory exposure assessment, was developed. In GeoPEARL, all processes which describe pesticide behaviour in the soil-plant system are simulated by the PEARL model. They are depicted in chapter 3.3.1. Instead of one single worst-case scenario, GeoPEARL uses several thousands of climate and weather scenarios. These scenarios represent the entire range of conditions in agricultural used regions of the Netherlands. The set up of the Dutch scenarios is shortly described in chapter 3.3.2.2 and chapter 3.3.2.3. For each scenario, PEARL model runs can be carried out and results can be visualised and analysed in maps. Therefore, GeoPEARL represents a tool for spatial modelling.

The goal of GeoPEARL is to provide a wide range of scenarios and to manage the input, the simulation and the output by the software. GeoPEARL is available with two user interfaces. The graphical user interface (GUI) can be used for the Dutch standard approach. It is convenient for the user because he can parameterise the simulation runs easily and the software manages all calculations and prepares the results, i.e. maps and graphs. The command line version of GeoPEARL requires more knowledge because the user must specify many of the parameters manually as well as performing the output-processing. However, the command line version can be adapted to other countries or regions using other spatial schematisations. Thus, it is more flexible.

GeoPEARL can improve the evaluation procedures within the process of pesticide registration by providing information on the spatial pattern of leaching behaviour. In the former Dutch registration procedure, decisions were based on the 80th percentile concentration in time (see chapter 3.1.2). Using the new modelling tool, decisions can be based additionally on the leaching concentrations in the potential area of use. The potential area of use is defined by the cultivated area of the crops of intended pesticide use. Information on the cropping area is included in the modelling software. For the simulation runs, only such scenarios are selected where the respective crop is grown. Thereby, unrealistic scenarios with respect to the intended use pattern can be excluded. The simulated concentration value which is used for the decision support is therefore a percentile of the concentrations in time as well as a percentile of the concentrations in the cultivated area. In the Dutch decision approach, that means that registration is only possible if the 50th percentile of the leaching concentrations for each scenario do not exceed the trigger value in 90 % of the area of potential use.

Therefore, GeoPEARL represents an important improvement of the decision support in pesticide registration due to the implementation of the spatial pattern of pesticide leaching behaviour. Nevertheless, the authors (Tiktak et al., 2003) advise the user against misinterpretation of the modelling results. Aside from the uncertainties of the PEARL model itself (see Leistra et al., 2001), the calculated maps should be handled with care. They seem to give accurate results of the leaching amounts in the groundwater whereas the spatial resolution and the data sources do not allow such precise predictions.

3.3.2.2 Spatial schematisation

The core of GeoPEARL is the spatial schematisation, i.e. the set of scenarios which is provided by the application. It was derived from a range of existing datasets with the help of GIS and methods of geoinformatics. In the following sections, the development of the schematisation and its parameterisation is described, based on the information given in Tiktak et al. (2003, 2004a).

The spatial schematisation was developed on the basis of the raster data model with a resolution of 250 m x 250 m. Each raster cell was assigned the parameters of the input maps. All raster cells that show the same combination of input data represent a single unique combination referred to as “plots” in the Dutch approach. Spatial information on the soil type, the land use type, the climate district, the hydrotype, drainage characteristics, seepage fluxes and the groundwater depth class were used as input data (see Figure 6).

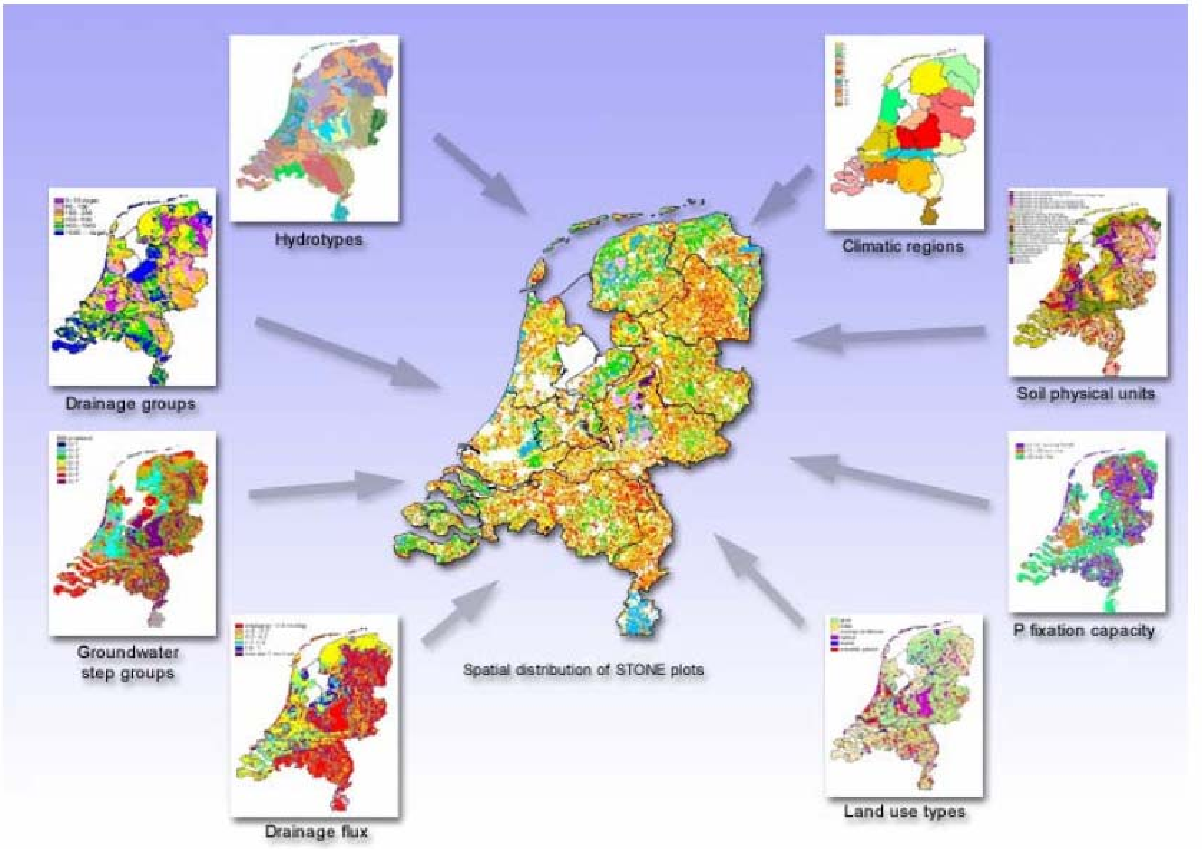


Figure 6: **Input data sets for the spatial schematisation of GeoPEARL (Tiktak et al., 2003)**

The combination of the input data sets using spatial overlay procedures led to a scenario number of more than 100,000. The computation time of such a large number of plots is unacceptable. The elimination of small sized combinations with similar attributes results in a more convenient calculation time without losing important information. Therefore, the number of plots was reduced to 6405 with the help of relation diagrams which give information on similar combinations to which the eliminated raster cells were assigned. An investigation on the quality of the resulting schematisation was carried out and it was decided that it was acceptable.

As the computation time for all plots is still very long, some approaches were developed to provide modelling results in a short time period. First, the software was adopted to be run on a grid, i.e. a network of a large number of computers, which reduces total computation time to a few hours. In addition, a method for further reduction of the calculated unique combinations was developed which can be carried out by the user. Thereby, plots whose simulation results are similar are merged together and only one single model run is conducted for them. The number of plots can just be reduced to the point where the results of GeoPEARL for decision support are not significantly influenced. However, this method requires a large number of model runs with various substances and crop scenarios to identify unique combinations which have similar modelling results.

3.3.2.3 Parameterisation of GeoPEARL

Each unique combination was assigned the parameters that are required for model input in PEARL. In the GUI-version, the spatial distributed parameters are stored in a relational database, in the command line version in text-files. Figure 7 shows the structure of the GeoPEARL database and the information which is provided.

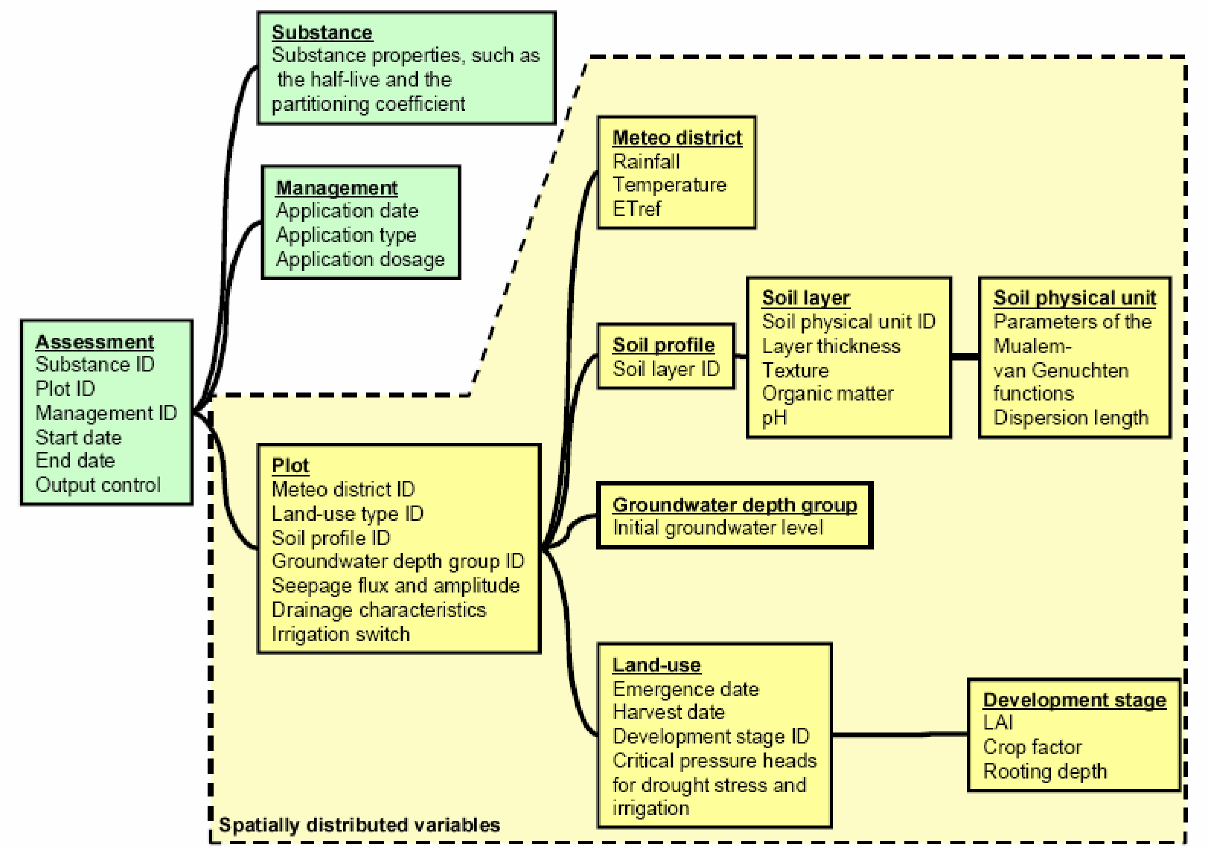


Figure 7: Structure of the GeoPEARL database (Tiktak et al., 2003).

For the Dutch schematisation, the following data sources were used:

Climate:

Daily data on maximum and minimum temperature, precipitation amount and reference evapotranspiration were obtained from 15 weather stations which were assigned to the 15 weather districts used for the spatial schematisation. A time series of 20 years was available for each station. Irrigation was assigned by expert judgment. The provided parameters are sufficient for model simulations. The additional climate parameters given in chapter 3.3.1.2 are required if the evapotranspiration is not available. Then, solar radiation, wind speed and air humidity can be used to derive the evapotranspiration values. The assumption that one weather station should be representative for a whole weather district is a critical issue of the Dutch schematisation.

Soil:

The soil parameters were taken from the Dutch soil map (1:50,000) and the related National Soil Database which provides about 4,500 soil profiles. Some parameters, such as the bulk density or the Mualem-van Genuchten parameters for soil hydraulic properties were derived using pedotransfer rules.

The values for the seepage flux were derived by the iterative adaptation of groundwater levels calculated by SWAP and by a regional hydrological model. The existence of a drainage system was obtained from expert judgment whereas the drainage characteristics were derived from topographical maps and the map of hydrotypes.

Land use:

The information on the land use was obtained from data of the Netherlands Statistical Bureau and from satellite images (Landsat). Information on 24 different crops is provided in the GeoPEARL database.

3.3.3 The EuroPEARL approach

The concept of GeoPEARL was transferred to the European scale by Tiktak et al. (2004b). The European spatial schematisation is called EuroPEARL. The application was developed in the context of the APECOP project of the European Union which gives guidance to the harmonisation of pesticide registration in Europe. The spatial schematisation of Europe consists of 1062 unique combinations, which were derived by overlaying soil data and climate data. Spatial information on soils was obtained from the Soil Map of Europe, which provides 735 soil mapping units. A climate map with eight European climate zones was used for the description of the weather conditions. The map is based on long-term averages of annual precipitation and temperature from about 1500 weather stations. Information on soil profiles is provided by the Soil Profile Analytical Database of Europe (SPADE1) containing 621 estimated soil profiles. The MARS database was used to obtain daily weather data. In the spatial schematisation, additional data such as irrigation or crop management were included. The spatial resolution of EuroPEARL is 10 km x 10 km according to the EU soil map. The spatial schematisation for Europe represents about 75 % of the total agricultural area in the European Union. Due to the lack of appropriate soil profile data for Austria, Sweden and Finland, these countries could not be considered for EuroPEARL.

Tiktak et al. (2004b) carried out model runs with four so-called dummy substances which were developed for test runs in the FOCUS context. They do not represent real active ingredients but show realistic parameter combinations. The results show that, generally, high leaching rates are correlated with high precipitation and irrigation and low organic matter contents. The authors advise to consider the results as real leaching concentrations at the respective place. Due to the coarse resolution and the insufficient data for several parameters, the described approach is only a first attempt for a pan-European consideration.

4 Materials and Methods

In the following sections, the generation of the German spatial schematisation for GeoPEARL_DE is described. First, an overview of the data sets used is given and the general procedure for the derivation of unique combinations and their parameterisation is outlined.

4.1 Spatial data sets

4.1.1 Overview of the used data sets

Land use

- CORINE land cover 2000 (ETC, 2006)
- Administrative units of Germany (BKG, 2005)
- Statistical data sets of crop cultivation (Federal Statistical Office of Germany, 2005)

Climate

- MARS data (50 km x 50 km tiles) (JRC, 2006b)
- DWD data (long-term values of temperature and precipitation, 1 km x 1 km raster) (DWD, 1999 - 2003, 2007)

Soil

- BÜK 1000 Germany (BGR, 2005, 2006)

4.1.2 Spatial reference system

For the combination of the different spatial data sources, a common spatial reference system is required. The German Gauss-Kruger-System was chosen with the parameters provided by the ArcGIS 9.1 ™ software (ESRI, 2005). The Gauss-Kruger-System (GK) is the projected coordinate system which is used in general for many datasets in Germany, especially for the official datasets such as topographic and thematic maps. The GK-system is based on the geographic coordinate system (GCS) "Deutsches Hauptdreiecksnetz" (DHDN). The meridian of 9° east is used as reference meridian. The used projection parameters are shown in Table 4.

Table 4: Parameters of the Gauss-Kruger projection (ESRI, 2005)

Projected Coordinate System: Gauss-Kruger Zone 3		
Parameters	Projection	Gauss-Kruger
	False Easting	3500000.000000
	False Northing	0.000000
	Central Meridian	9.000000
	Scale Factor	1.000000
	Latitude of Origin	0.000000
	Linear Unit	Meter (1.000000)
Geographic Coordinate System	Name	GCS_Deutsches_Hauptdreiecksnetz
Parameters	Angular Unit	Degree (0.017453292519943299)
	Prime Meridian	Greenwich (0.000000000000000000)
	Datum	D_Deutsches_Hauptdreiecksnetz
	Spheroid	Bessel_1841
	Semimajor Axis	6377397.155000000300000000
	Semiminor Axis	6356078.962818188600000000
	Inverse Flattening	299.152812799999990000

4.1.3 The CORINE land cover data set

In the 1980s, the European Commission decided to develop a comprehensive spatial database including various data sets on environmental parameters which is called CORINE (Coordination of Information on the Environment, Mounsey, 1991; EEA, 2004; JRC, 2006a; European Topic Centre on Terrestrial Environment, 2006). One part of the new database is a pan-European map of land use. The CORINE land cover (CLC) data set describes the land use of Europe in a harmonised way on the basis of remote sensing data without semantical breaks. The first version of CLC was published in 1990. Within the CLC 2000 project, the data were updated using satellite imagery data from 1999 to 2000. The European Environment Agency and the European Topic Centre for Terrestrial Environment were responsible for project management and coordination. The interpretation of the image data was carried out by the national authorities on the basis of satellite images, i.e. the ETM+ Landsat 7 satellite.

44 land use classes are defined which follow a system with three hierarchical levels. For the first level, five classes are available: artificial surfaces, agricultural areas, forests and semi-natural areas, wetlands, and water bodies (see Table A 1). Figure A 1 shows a map of the CLC 2000 data set. For the development of the spatial schematisation of GeoPEARL_DE, the information on agricultural areas (see Table 5) was used to focus on the relevant regions that define the area of interest for GeoPEARL_DE (see chapter 6). Additionally, core regions of vine and orchard cultivation are identified using the CLC data set (see chapter 5.3.3).

Table 5: CLC classes defining agricultural land use

CLC code	Class definition
211	Non-irrigated arable land
221	Vineyards
222	Fruit trees and berry plantations
231	Pastures
242	Complex cultivation patterns
243	Land principally occupied by agriculture, with significant areas of natural vegetation

The CLC data set is available in the vector shape format and in the raster format with different resolutions (100 m, 250 m or 1000 m) via the online data service of the European Environment Agency. For the spatial schematisation, the 1 km x 1 km raster data set from 2000 was used because its scale corresponds with the scale of the other data sets. Additionally, it is congruent to the raster data set presenting long-term climate data of the German weather service (see chapter 4.1.7).

4.1.4 The administrative units of Germany

The administrative units of Germany are provided by the German “Bundesamt für Kartographie und Geodäsie” (BKG) (BKG, 2005). The data set includes the objects of each administrative level in Germany such as the federal states, rural districts, and communities. They are represented by vector data. The data set used shows the status of the boundaries at reporting date 31-12-2004. Figure A 2 shows a map of the administrative units.

4.1.5 German crop statistics

Information on the cultivated area in Germany is available in the German crop statistics which are provided by the Federal Statistical Office of Germany (2005). Regarding the area with agricultural land use, the following items are available:

- Total agricultural area including field crops, permanent crops and pastures
- Field crops including cereals, root crops, forage plants and industrial crops
- Cereals including wheat, rye, winter barley, spring barley, oat and triticale
- Root crops including potatoes and sugar beets
- Forage plants including silage maize
- Industrial crops including winter oil seed rape.

The data on the cultivated area are available for different levels of administrative units, i.e. from community level up to the level of the federal state and Germany as a whole. The data can be linked to the data set of the administrative units via an ID and can be analysed or visualised in maps. The crop statistic data were used to set up the crop area database of GeoPEARL_DE.

4.1.6 The MARS weather data set

In 1988, the Joint Research Centre (JRC) of the European Commission started a project to monitor agriculture with space technologies – MARS (**M**onitoring of **A**griculture with **R**emote **S**ensing). Within the MARS project, a Crop Growth Monitoring System (CGMS) is embedded. Spatial data on weather indicators, crop indicators, vegetation indices and cumulated dry matter are provided (JRC, 2006c). For the derivation of GeoPEARL_DE, the meteorological information of the MARS database was used. According to the MARS project, the weather data are called “MARS data”. The MARS data are available for a 50 km x 50 km raster covering the whole of Europe and for time series since 1975. For each raster cell, several daily weather parameters are provided which were generated by interpolating data from European weather stations to the raster cells. The geometry of the raster as well as the weather data themselves are available via the JRC MARS homepage (JRC, 2006b). The format of the geometry data is the vector format represented by a shape file with square polygons, the weather data are provided in text-files. Their distribution is restricted to authorised users.

GeoPEARL requires daily weather data for the simulations which are provided by the MARS data. For the spatial schematisation of GeoPEARL_DE, the data sets of the years 1992 to 2004 were used. Information is provided for the following parameters:

- Date
- Daily maximum of temperature (°C)
- Daily minimum of temperature (°C)
- Daily amount of precipitation (mm)
- Penman potential evaporation from a free water surface (mm day^{-1})
- Penman potential evaporation from a moist bare soil surface (mm day^{-1})
- Penman potential transpiration from a crop canopy (mm day^{-1})
- Daily global radiation (KJ m^{-2})

Figure A 3 shows a map of the MARS tiles covering Germany.

4.1.7 The DWD weather data set

Spatially distributed long-term values of temperature and precipitation are available in the “Klimaatlas Deutschland” (DWD, 1999 - 2003). The digital data set is provided by the German weather service (Deutscher Wetterdienst, DWD) for data analysis. The data set contains long-term average values of the temperature and the rainfall for each month. The data were collected during a 30 years time period from 1961 to 1990. They are provided in the ASCII raster format with a cell size of 1 km x 1 km (DWD, 2007) which is congruent to the raster version of the CORINE land cover. 24 raster data sets are available, twelve representing the precipitation data (one for each month) and twelve representing information on the temperature (one for each month). As the data set represents a spatial resolution which is appropriate for the purposes of GeoPEARL_DE, it is used in combination with the MARS data set to generate a new data set with high spatial as well as high temporal resolution (see chapter 8.4). Figure A 4 and Figure A 5 show maps of the precipitation and the temperature data sets. Here, combined information, i.e. the annual sum of precipitation and the annual mean of temperature, is presented.

4.1.8 The German soil database

The soil map

The soil map 1:1,000,000 (Bodenübersichtskarte (BÜK) 1000) of Germany provides generalised spatial soil data for Germany (BGR, 2005, 2006). The legend units of the map represent a combination of the soil unit, the climate region, the land use, and the “Bodengroßlandschaft” (BGL), a level for aggregation of soil units in Germany.

The soil unit is defined as a so-called “Leitbodenassoziation” (LBA). It is an aggregation level considering parameters of the soils and the substrate. Soil units covering only small areas were eliminated. The LBA is a lower aggregation level than the BGL. The information of the climate region was derived from the European soil database (JRC, 2003). The land use information was taken from the CORINE land cover data collected in 1990. The CLC data were generalised and adapted to the German soil map. Figure A 6 shows a map of the BÜK data set. The soil map was used for the development of the spatial schematisation.

The soil profiles

The BÜK database provides a set of soil profiles which can be related to the legend units. In general, for each legend unit, soil profiles for the following land uses are included:

- Agricultural land use
- Pastures
- Forest

Soil profiles are not available for each combination of legend units: Some legend units exclude certain land uses (e.g. “settlements”) or a soil profile is not yet defined by the BGR. Table 6 represents the soil units which exclude agricultural land use by their definition. Table 7 and Table 8 show the legend units for which no soil profiles “agricultural land use” or “pastures” are defined by the BGR.

Table 6: BÜK legend units excluding agricultural land use

Climate region	Description	Soil unit	Short description
33	Temperate sub-oceanic climate	2	Tide lands
		70	Settlements
		71	Areas influenced by men (dumps, extraction sites)
		72	Water bodies
34	Temperate sub-oceanic to temperate sub-continental climate, mountain climate in parts	70	Settlements
		71	Areas influenced by men (dumps, extraction sites)
		72	Water bodies
35	Temperate sub-continental climate	70	Settlements
		71	Areas influenced by men (dumps, extraction sites)
		72	Water bodies
38	Temperate mountain climate	69	Lithic Leptosols
		72	Water bodies

Table 7: BÜK legend units without soil profiles “agricultural land use“

Climate region	Description	Soil unit	Short description
33	Temperate sub-oceanic climate	59	Shallow, acid, brown soils
34	Temperate sub-oceanic to temperate sub-continental climate, mountain climate in parts	33	Shallow, dry, often acid, sandy soils
		38	Deep black earth
		62	Shallow, sandy soils in the Hunsrück and Taunus
35	Temperate sub-continental climate	18	Shallow to deep, sandy-loamy, brown soils
38	Temperate mountain climate	06	Fen soils
		07	High moor soils
		10	Deep, sandy to sandy-loamy soils influenced by groundwater
		11	Deep, sandy soils influenced by groundwater
		14	Shallow, silty-loamy, brown soils
		21	Deep, loamy-sandy brown soils (moraine deposition)
		52	Clayey, silty or sandy-loamy, decalcified brown soils
		68	Heterogeneous structure of shallow, loamy-stony soils in the Alps

Table 8: BÜK legend units without soil profiles “agricultural land use“ and “pastures“

Climate region	Description	Soil unit	Short description
34	Temperate sub-oceanic to temperate sub-continental climate, mountain climate in parts	33	Shallow, dry, often acid, sandy soils
		38	Deep black earth
35	Temperate sub-continental climate	18	Shallow to deep, sandy-loamy, brown soils
38	Temperate mountain climate	14	Shallow, silty-loamy, brown soils

The description of the soil profiles includes the most important soil parameters according to the German guideline for soil description (AG Boden, 1994). For the parameterisation of GeoPEARL_DE, the following parameters were used:

- Number of horizon
- Symbol of horizon
- Upper boundary of horizon
- Lower boundary of horizon
- Soil texture (German classification)
- Bulk density (German classification)
- Organic matter (German classification)
- pH-value (German classification)

For the soil profiles related to agricultural land use, soil hydraulic parameters are provided by BGR (2006).

4.2 Tools and methods

For the development of GeoPEARL_DE, the command line version of the GeoPEARL software as described by Tiktak et al. (2003, 2004a) was used (see also chapter 3.3.2.1). The original application GeoPEARL is depicted in detail in the previous sections. For GeoPEARL_DE, only the spatial schematisation was changed as described in the following sections. The behaviour and the properties of the software using the German schematisation are discussed in chapter 9.

The German schematisation for GeoPEARL_DE was realised on the basis of a raster data set which is convenient for generation of the schematisation and for further processing, visualisation and dissemination of the simulation results. Furthermore, raster data sets are easy to handle during spatial analysis. For GeoPEARL_DE, a 1 km x 1 km raster data set was chosen as the basic raster. This raster is congruent to the spatial data sets of the German weather service (DWD) and the CORINE land cover (see chapter 4.1.3 and 4.1.7). The cell size, the scale and the projection of the data are considered as appropriate regarding the German situation and the purpose of the application.

From the basic raster data set, all cells which are not covered by agricultural land use, were eliminated to focus on the relevant land use. Thereby, environmental parameters such as extreme weather conditions which do not emerge in cultivated areas can be excluded from the parameterisation. The resulting data set represents the area of interest for GeoPEARL_DE. The raster cells of the area of interest were allocated to unique combinations of the relevant environmental parameters, i.e. climate and soil. The unique combinations were derived by overlay procedures. Different layers of environmental parameters (here: climate and soil) were combined and raster cells that show the same parameter set were allocated to the same unique combination. Each unique combination was then parameterised according to the requirements of GeoPEARL. Thus, a set of different environmental scenarios showing different properties of soil and climate exists. For each of the unique combinations, i.e. each scenario, a single model run can be carried out. Further processing of the results is then possible, e.g. maps can be created or further analysis can be conducted.

The spatial schematisation was created with the help of the GIS software ArcGIS 9.1^{TM} and the extension Spatial Analyst^{TM} (ESRI, 2001 – 2005). For calculations, data transformations, handling and storage, the Microsoft Office software EXCEL 2003^{TM} and ACCESS 2003^{TM} were used. The generation of the unique combinations, as well as parts of the parameterisation procedure, were carried out with the help of GIS-procedures as overlay, raster calculations, or zonal statistics.

5 Data preparation

All data sets were projected to the common projected coordinate system “Gauss-Kruger” which is described in chapter 4.1.2. For the MARS data set and the BÜK map, transformation procedures are required. Beside retransformation, the following data sets need further preparation:

- CLC: Definition of a mask focusing on agricultural land use
- Administrative units: Selection of one single level for each federal state
- Crop statistics: Data processing
- DWD: Generation of two raster data sets representing annual mean of temperature and annual sum of precipitation
- BÜK: Generation of new code as a combination of climate region and soil unit

5.1 Preparation of the CORINE land cover

As GeoPEARL simulations focus only on regions with agricultural land use, an area of interest was defined on the basis of the CORINE land cover data set. Therefore, the CLC data set was manipulated. All raster cells were reclassified in two classes – one contains the cells classified as agricultural land use, whereas the second class contains all other land uses. Agricultural land use is defined by the CLC codes shown in Table 5.

Information on land use in Germany is available both by the CLC data set and by the BÜK database. The land use information of the CLC data set is used for the schematisation procedure because the information in the BÜK data set is ten years older than in the CLC 2000 data set. It was derived from the CLC data set gathered in 1990.

5.2 Preparation of the administrative units

The different administrative levels of Germany were reduced to one single level for each federal state based on the criterion of completeness of crop statistical data as provided by the Federal Statistical Office of Germany (2005) on the respective levels. This step is required to join the statistical data to the administrative units (see chapter 5.3). For most federal states, rural districts were selected. For North Rhine-Westphalia, the level of the communities were chosen and for Hamburg and Berlin, the level of the federal state. These polygons were merged together creating a new data set that is used for the adaptation of the statistical data on cropping area (see chapter 8.3.2).

5.3 Preparation of the statistical data set

5.3.1 Standard crops

The data on the land use area are available for different levels of administrative units. The lowest level is the level of the community. For many of the communities, the required data are missing. Hence the next level was used for the investigation: the rural districts which represent an appropriate resolution for the application regarding the other spatial data sets. For some rural districts, certain data are not reported in the database for privacy reasons. Missing values were then estimated on the basis of the federal states where information on all data is available. For North Rhine-Westphalia, the data for the communities are complete. They were used for the investigation.

5.3.2 Maize data

The crop “maize” is not completely listed in the database. Only the area of silage maize is provided. The area of corn and corn-cob-mix is included in the total area of the field crops. The total area of maize was derived using two methods. First, the sum of the area of all subsets of cereals was subtracted from the total area of cereals. This value represents the area of corn and corn-cob-mix. It was added to the value of the area of silage maize. The area of maize is overestimated using this method. For the second method, additional data of corn-cob-mix for each rural district in Germany (Statistische Landesämter, 2005) are available. The provided values were added to the area of silage maize. For North Rhine-Westphalia, the additional data set was not used because for this federal state data on the community level were available. The user can select between the two data sets for maize for model simulations.

5.3.3 Data of orchards and vine

In the data set of the Statistical Office, the data for orchards and vine were not listed separately. They were included in the parameter “permanent crops”. By using the values of this parameter instead of the real values of orchards and vine, the cropping area of these two crops would be overestimated considerably. Hence, the CORINE land cover data set was used to specify the cropping area. In the CLC data set, these two crops are listed separately (CLC classes 2.2.1 (vine) and 2.2.2 (orchards)). The spatial information of CLC and the statistical data set were combined and the cropping area of orchards and vine were determined in a more exact way using the following rules:

- If an administrative unit was covered by orchards as derived from the CLC data set, the area of permanent crops was assigned to orchards.
- If an administrative unit was covered by vine as derived from the CLC data set, the area of permanent crops was assigned to vine.
- If an administrative unit was covered by both orchards and vine, the area of permanent crops was assigned to orchards and vine considering the ratio of orchards and vine in the CLC data set.
- If an administrative unit was covered neither by orchards nor vine, the area of permanent crops was not considered and the area of vine and orchards was set to zero.

5.4 Preparation of the DWD data set

The DWD data set represents the monthly mean temperature and the monthly sum of precipitation. For the derivation of the schematisation, the annual mean temperature and the annual sum of precipitation were required. The twelve raster data sets representing the monthly means of precipitation were summarised to a single raster in order to obtain the annual sum of precipitation. The raster showing the annual mean temperature was calculated from the twelve monthly raster data sets as the weighted mean of the monthly mean temperatures with the number of days as weighting factors.

5.5 Preparation of the soil database

As described in chapter 4.1.8, the BÜK legend units represent a combination of soil unit, climate region, land use, and BGL. Two of these items were ignored: Land use information was derived from the CLC database (chapter 5.1). The item "BGL" is not required. Thus, the information of the BÜK map is reduced to the combination of the soil unit and the climate region. The soil unit of the BÜK is composed of 72 different items. Additionally, four climate regions are implemented in the BÜK data set. The spatial combination of the soil unit and the climate region leads to 157 items. The 157 combinations are called "soil code". The soil code is composed of the ID for the climate region and the ID for the BÜK soil unit.

For most of the BÜK legend units, a soil profile with agricultural land use is available in the soil profile database which is used for the parameterisation of GeoPEARL_DE. For some legend units, respective profiles are not available as shown in Table 6. The legend units which exclude agricultural land use (e.g. settlements) were excluded from the area of interest (see chapter 6). They were not considered for the generation of the spatial schematisation. So, 145 combinations of soil unit and climate region which can be used for model parameterisation remain. The legend units for which the BGR do not provide adequate soil profiles were not excluded from the area of interest. However, the resulting unique combinations were not parameterised and they were excluded from model calculations. Thereby, a later parameterisation is possible if new soil profiles become available.

6 Development of the area of interest

The spatial schematisation of GeoPEARL_DE was set up on the basis of a 1 km x 1 km raster which is congruent to the raster of the DWD data and the CORINE land cover. As basic raster, the DWD raster data set was chosen. For the model simulations, only the raster cells covered by agricultural land use were required – the area of interest. Thereby, environmental parameters, such as weather conditions, which do not occur in cultivated areas, can be excluded from the parameterisation. The land use information is included in the CORINE land cover data set. Thus, in the basic raster data set, the cells without agricultural land use as defined by the CLC data set were eliminated. Afterwards, the raster cells that are not covered by agricultural land use in the BÜK data set were removed. This step is necessary to avoid raster cells that cannot be assigned to a soil profile because they are covered by non-agricultural land use according to the BÜK 1000 data set. The land use information in the BÜK data set differs from the CLC 2000 data set due to spatial generalisation and the different reporting dates. Figure 8 shows the workflow for the derivation of the area of interest.

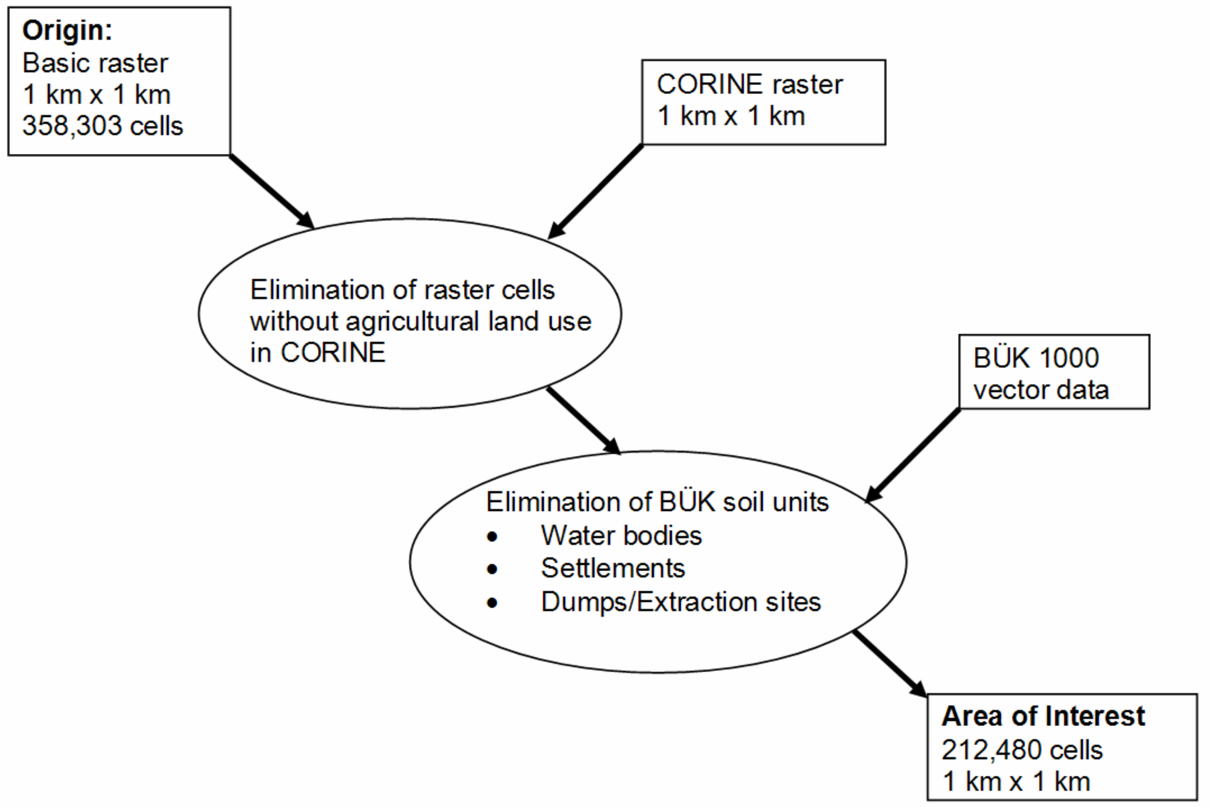
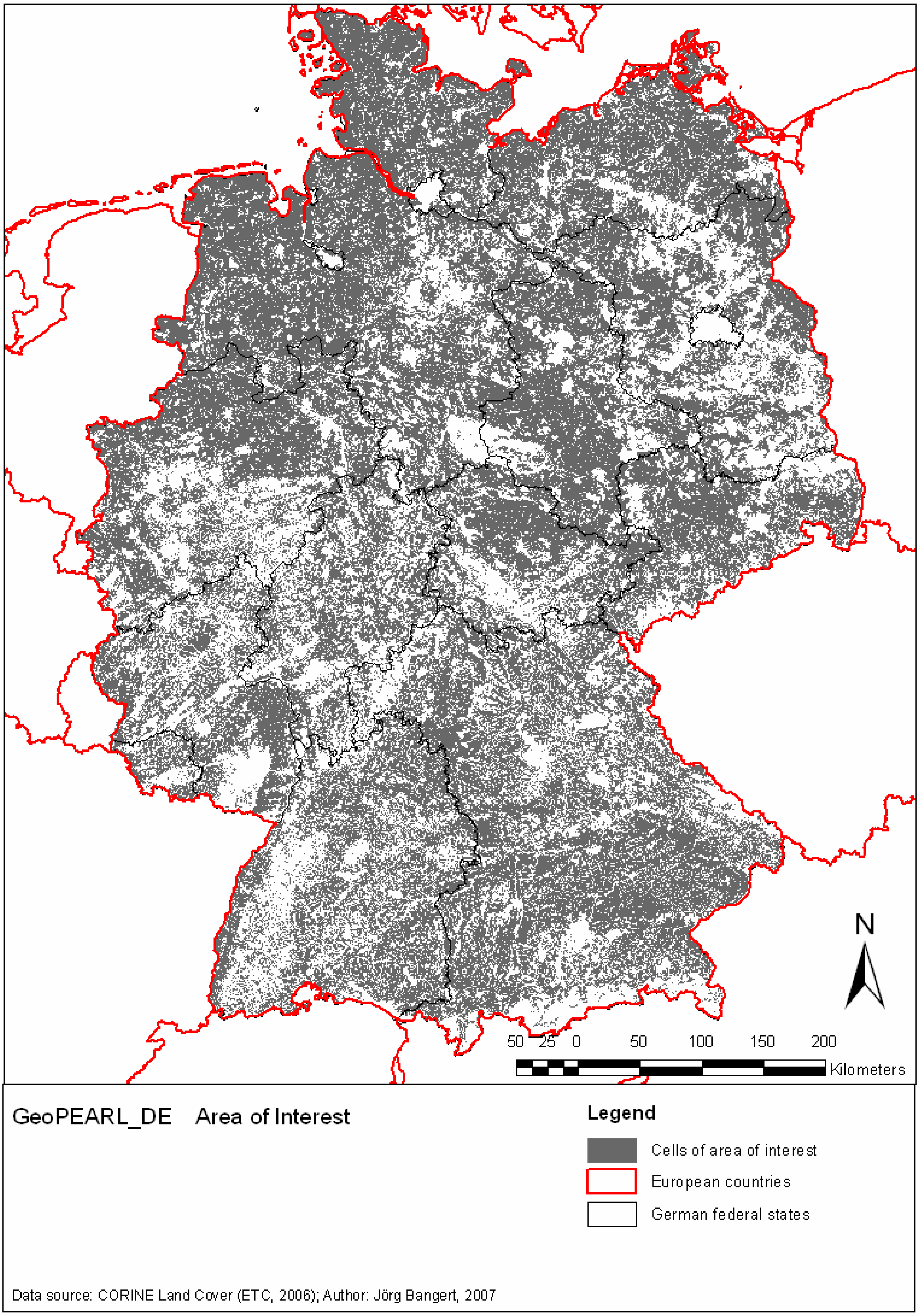


Figure 8: Workflow for creating the area of interest

The CORINE land cover raster was prepared by generating a mask as described in chapter 5.1. From the resulting raster, the cells which are covered by one of the BÜK soil units excluding agricultural land use (see Table 6) were eliminated. The remaining number of raster cells used for the German schematisation is 212,480. The output raster data sets represent the area of interest for GeoPEARL_DE which is shown in Figure 9.



Data source: CORINE Land Cover (ETC, 2006); Author: Jörg Bangert, 2007

Figure 9: **The area of interest for GeoPEARL_DE**

7 Derivation of unique combinations

GeoPEARL_DE simulations are carried out for a set of environmental scenarios. Each scenario represents a spatial entity of given parameters for soil and climate. Such an entity is called “unique combination” (UC). Within a scenario, the environmental parameters are considered to be uniform. The unique combinations were derived by overlay procedures using the following three data sets:

- Long term values for precipitation and temperature (DWD data)
- Daily weather information (MARS data)
- Information on soils (BÜK data)

The DWD data set provides only long-term climate values but shows a sufficient spatial resolution regarding the purpose of the model. On the other hand, the MARS database provides a high temporal but only a coarse spatial resolution. Both data sets were combined during the parameterisation process to get a data set with high temporal as well as high spatial resolution (see chapter 8.4).

The pattern of the unique combinations is called the spatial schematisation of Germany. This chapter describes the derivation of this pattern. In chapter 8, the parameterisation of the scenarios is explained. Figure 10 shows the workflow for the creation of the unique combinations starting with the area of interest that has been described in chapter 6.

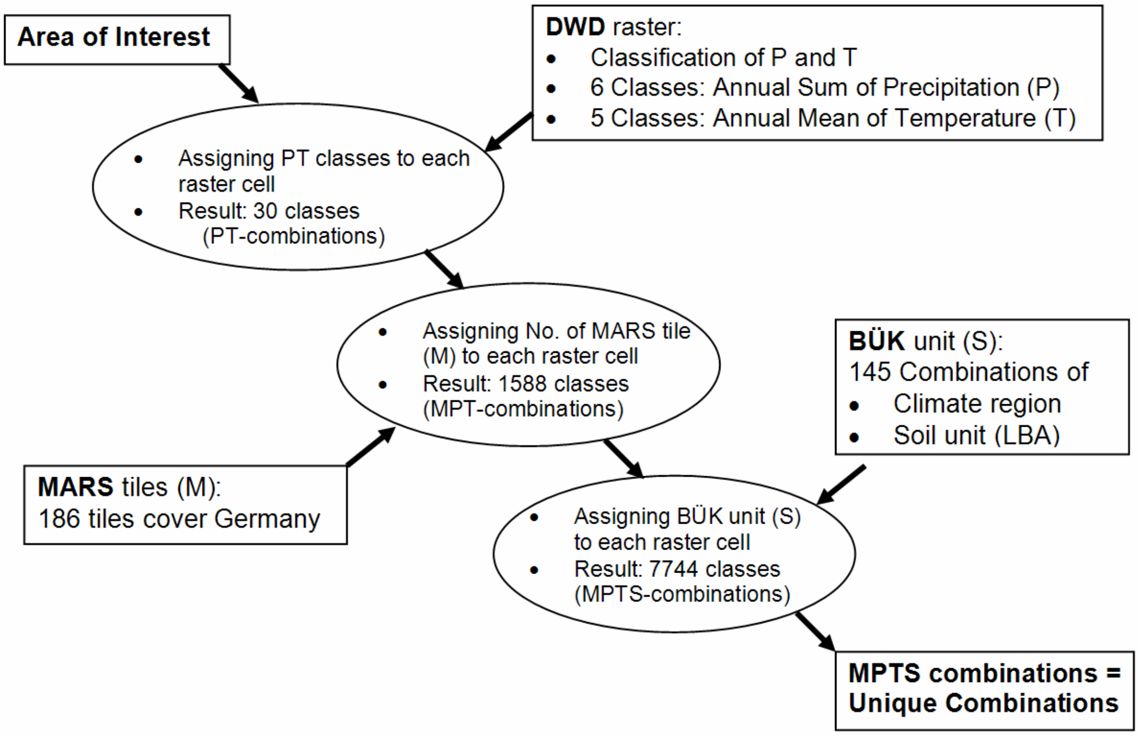


Figure 10: Workflow for generating the unique combinations

7.1 Classification of the weather data

Before carrying out the overlay procedure, the DWD data set was processed to focus on the required information level. The numerical values for temperature and precipitation were aggregated because the information is too complex for the GeoPEARL_DE approach. The data were classified as described in the following sections. The classification of the DWD data is based on the annual mean of temperature and the annual sum of precipitation for the 212,480 raster cells of the area of interest.

7.1.1 Classification of the temperature data

The distribution of the unclassified temperature data (annual mean) is shown in Figure 11 and Table 9.

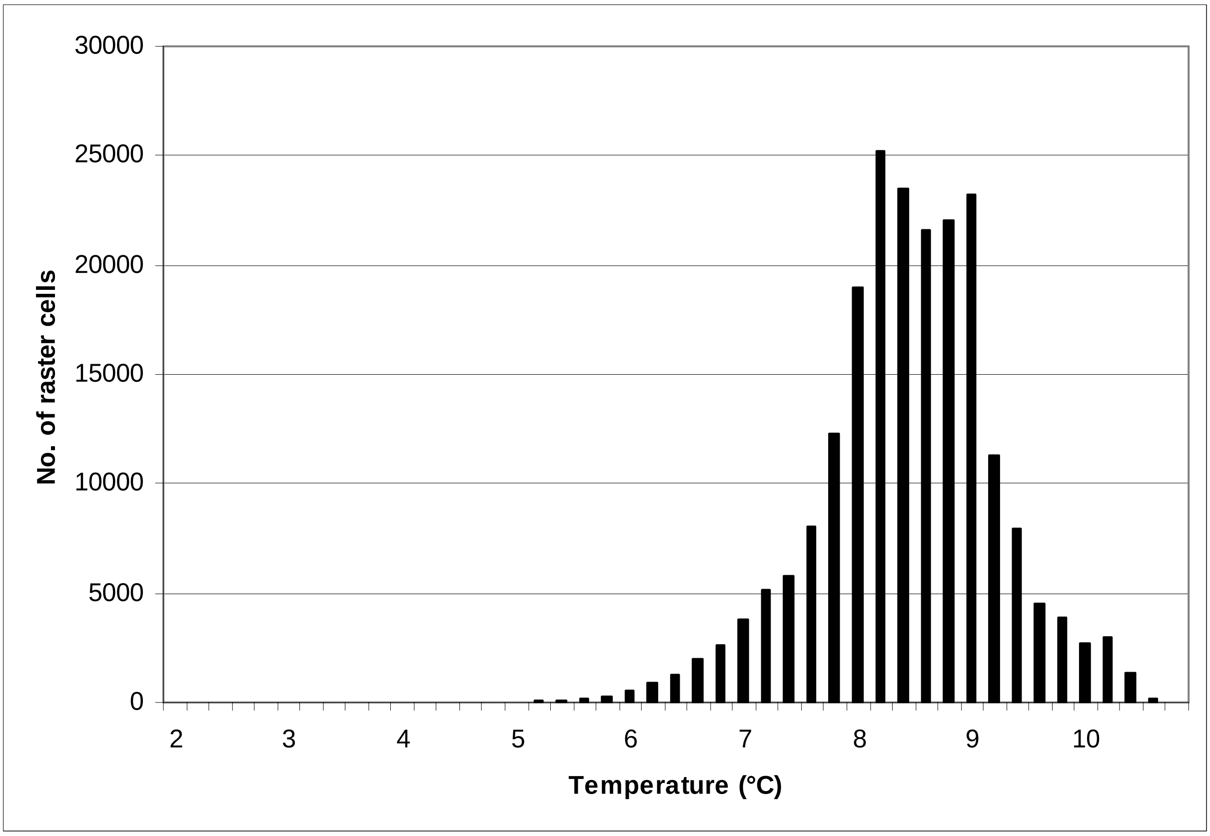


Figure 11: Distribution of the temperature data

Table 9: Statistical values of the temperature data

Number of raster cells	212,480
Minimum [°C]	1.9
Maximum [°C]	10.8
Mean [°C]	8.39

A classification by quantile with five classes was chosen for the temperature data. It was considered as appropriate because of the symmetry of the distribution of the temperature. The classes and their breaks are shown in Table 10.

Table 10: Classes of temperature

Temperature [°C]	Class code
0 – 7.8	1
> 7.8 – 8.2	2
> 8.2 – 8.6	3
> 8.6 – 9.0	4
> 9.0 – 10.8	5

7.1.2 Classification of the precipitation data

Step 1: 5 classes (quantile)

The distribution of the precipitation data is shown in Figure 12 and Table 11. The values are given in mm.

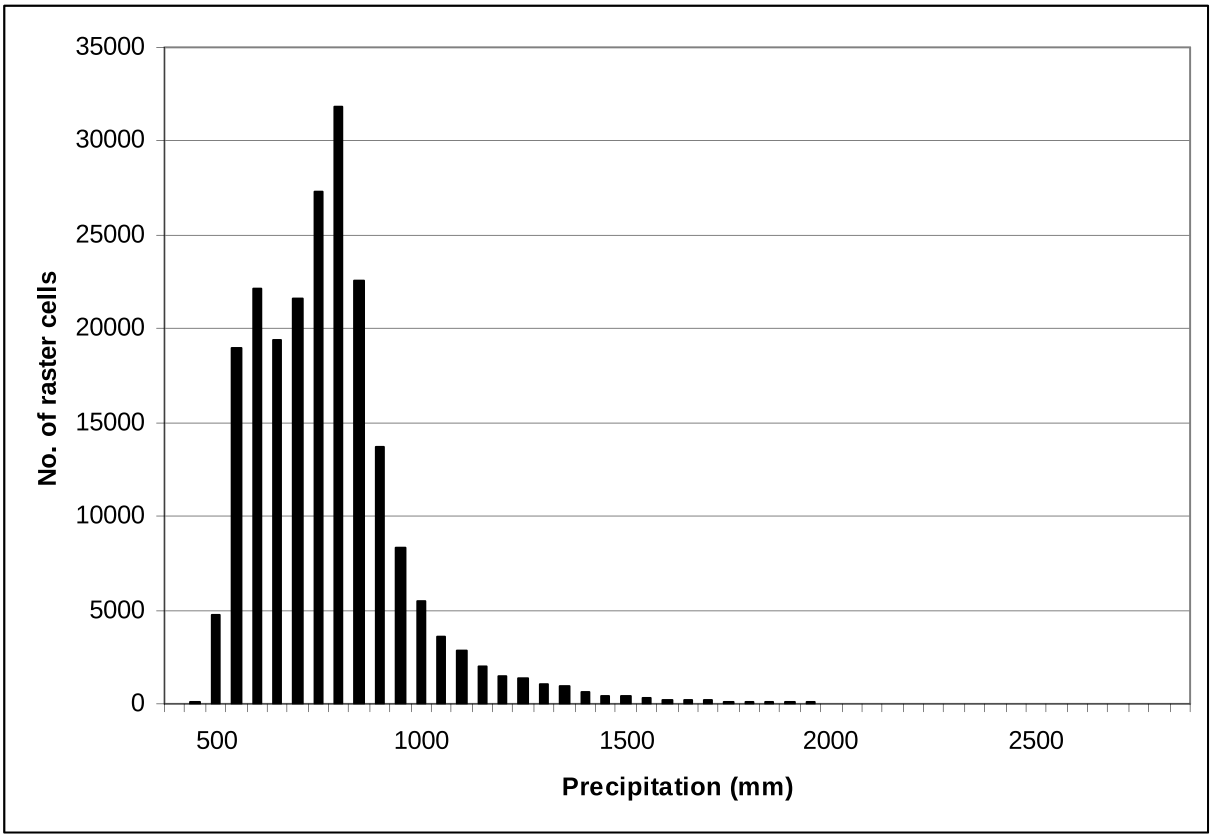


Figure 12: Distribution of the precipitation data

Table 11: Statistical values of the precipitation data

No. of raster cells	212,480
Minimum [mm]	384
Maximum [mm]	2854
Mean [mm]	751.22

In a first step, a division of the precipitation data into five classes by the quantile method was conducted. The class boundaries of this approach are shown in Table 12.

Table 12: Classes of precipitation (1st classification step)

Precipitation [mm]	Class code
0 – 591	10
> 591 – 696	20
> 696 – 769	30
> 769 – 855	40
> 855 – 2854	50

Step 2: Refinement of the basic classification

The combination of the data of temperature and precipitation (according to chapter 7.2) leads to a large number of raster cells in the class of high precipitation and low temperature as shown in Figure 13 and Table 13.

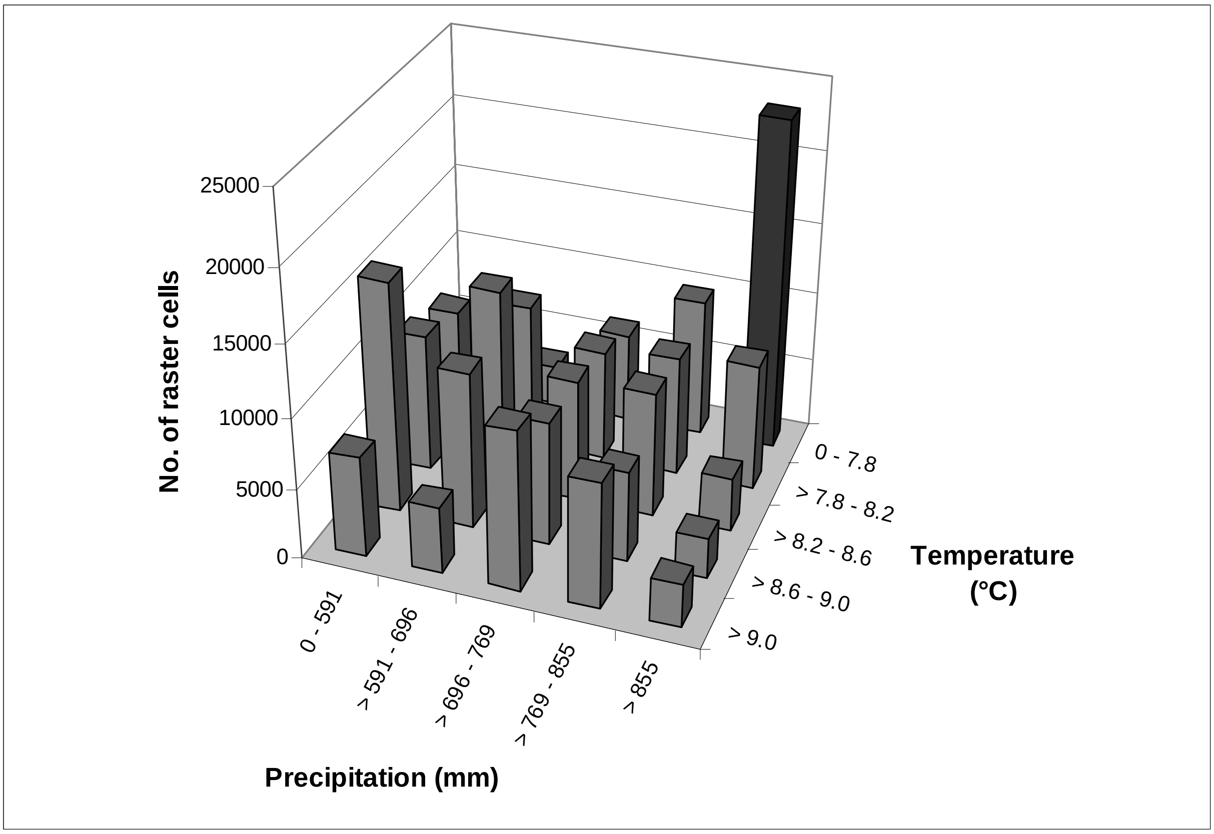


Figure 13: Distribution of the raster cells after combination of precipitation and temperature

Table 13: Number of raster cells per class after combination of precipitation and temperature

		Precipitation [mm]				
		0 - 591	> 591 - 696	> 696 - 769	> 769 - 855	> 855
Temperature [°C]	0 – 7.8	552	2910	6332	9767	**23348**
	> 7.8 – 8.2	8804	10113	7858	8483	8956
	> 8.2 – 8.6	9768	13941	8626	8867	3877
	> 8.6 – 9.0	16312	11052	8684	6346	2888
	> 9.0	7107	4688	11239	8918	3044

The combination of high precipitation and low temperatures is vulnerable for leaching. Furthermore, the range of the precipitation class is very large (855 mm – 2854 mm). Thus, a better differentiation and a refinement of the classification were required. Hence, a sixth class was introduced for the precipitation data. The new class boundary divides the previous fifth class in such a way that the combination class of low temperature and high precipitation was divided into two parts with a similar number of raster cells. The new break value between the fifth and the sixth class was defined at

994 mm. For the final classification, the break values were rounded to 0 or 5 at the last digit. In Table 14, the final classes and the break values are shown.

Table 14: Classes of precipitation (2nd classification step)

Precipitation [mm]	Class code
0 – 590	10
> 590 – 695	20
> 695 – 770	30
> 770 – 855	40
> 855 – 995	50
> 995 – 2854	60

7.2 *Creation of the PT combinations*

The spatial data sets including the precipitation (P) and the temperature (T) were combined in a spatial overlay procedure and the PT combinations were created. The PT combinations represent the first step towards the final set of unique combinations. Figure 14 and Table 15 show the number of raster cells in each PT combination. The number was considered to be suitable regarding the unfavourable input data, i.e. the skewed distribution of the precipitation data.

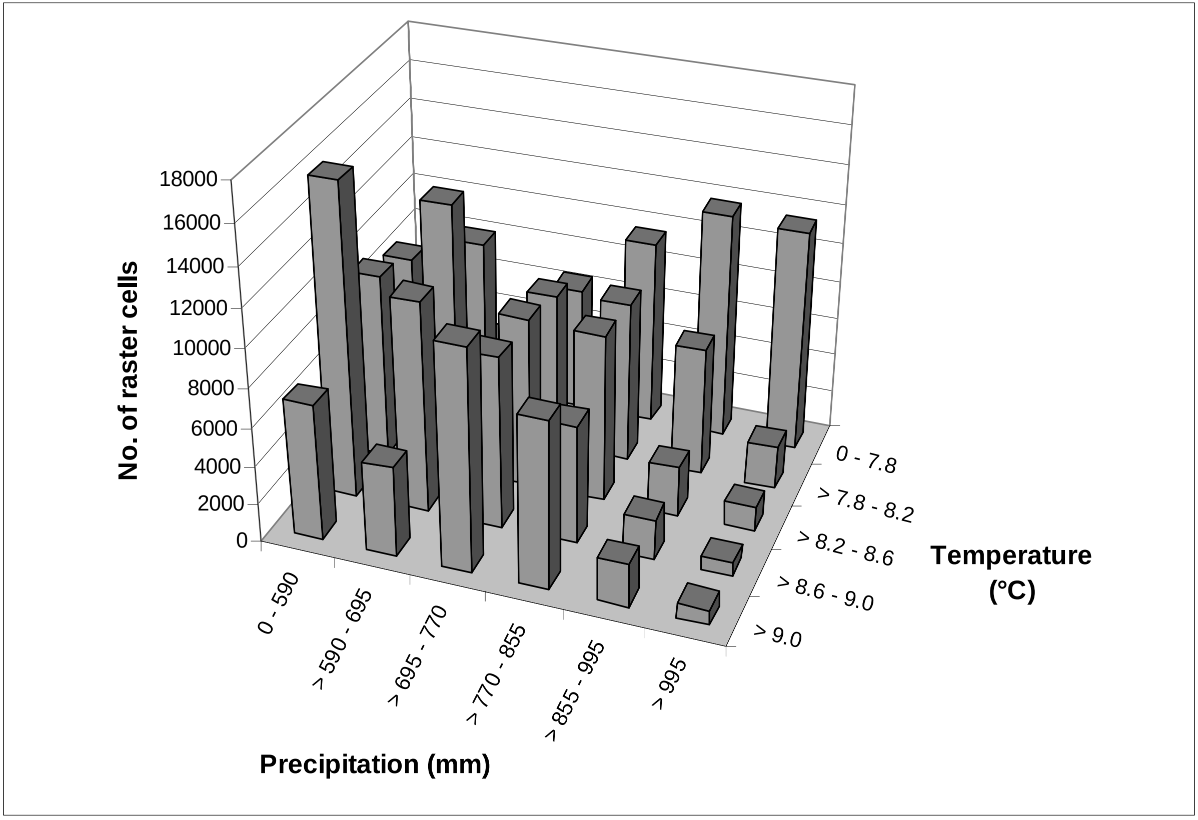


Figure 14: Distribution of the raster cells in the PT data set

Table 15: Number of raster cells in each PT combination

		Precipitation [mm]					
		0 - 590	> 590 - 695	> 695 - 770	> 770 - 855	> 855 - 995	> 955
Temp. [°C]	0 – 7.8	541	2873	6501	9646	11756	11592
	> 7.8 – 8.2	8672	10122	8083	8381	6694	2262
	> 8.2 – 8.6	9658	13957	8856	8731	2587	1290
	> 8.6 – 9.0	16232	11012	8943	6207	2141	747
	> 9.0	7075	4668	11521	8688	2249	795

Figure 15 shows the spatial distribution of the PT classes in Germany. Temperature is displayed with different colours. Different precipitation classes are displayed with different intensity of the colours. The legend of the map shows the ID of the respective PT class and the break values.

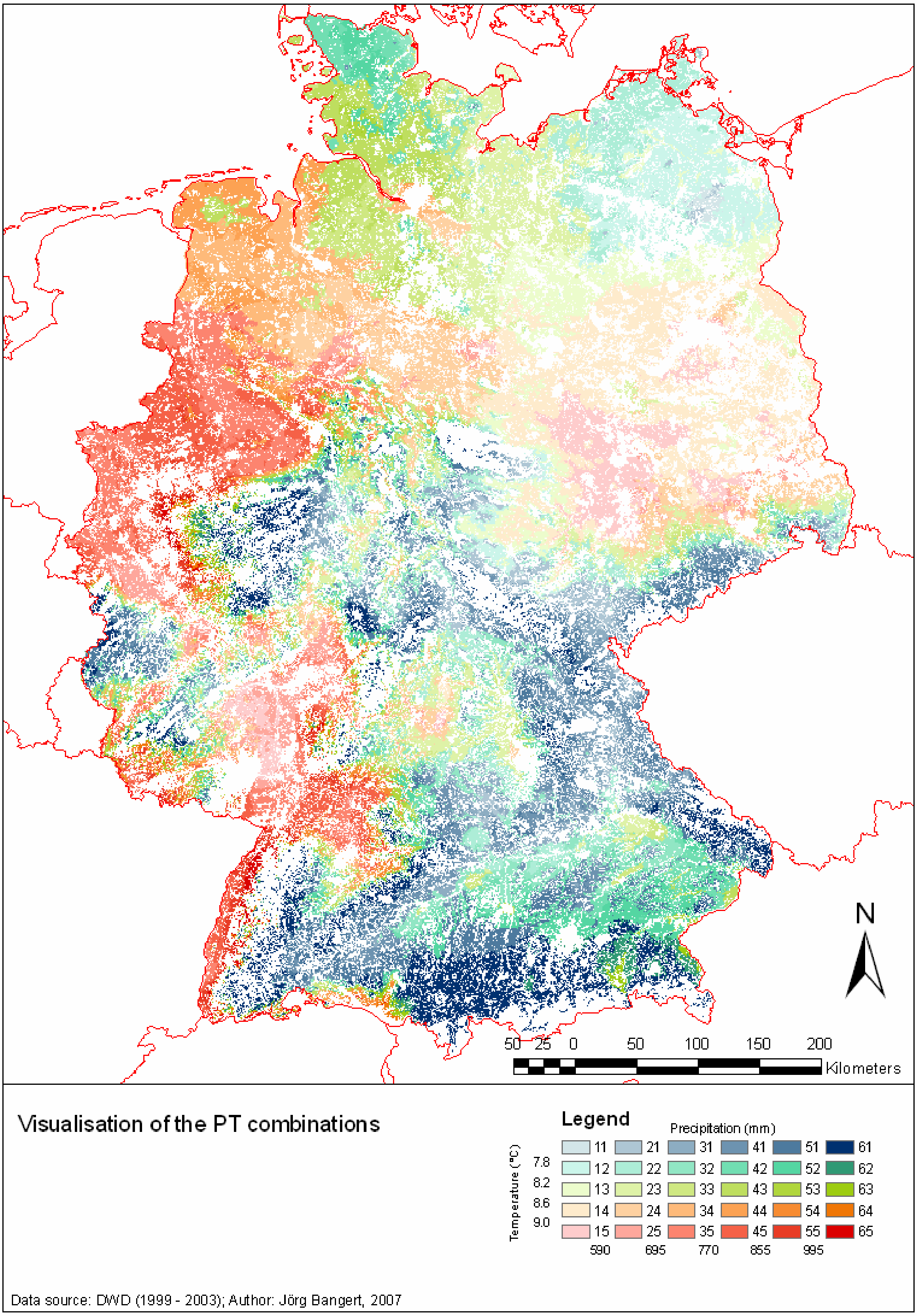


Figure 15: Spatial distribution of the PT combinations

7.3 *Creation of the MPT combinations*

After creating the PT combinations, the spatial information of the MARS tiles was allocated to the raster cells. For this purpose, the ID of each MARS tile was joined to the raster cells whose centre points are covered by the respective tile. The resulting combinations were called the MPT (**M**ARS **P**recipitation **T**emperature) combinations. The MARS ID was placed on the first position of the MPT raster value. Thus, the unique combinations of the final spatial schematisation can be ordered easily in the attribute table by their spatial neighbourhood. This is an advantage for setting up model calculations in a special GeoPEARL_DE mode. The new raster data set includes 1588 MPT combinations. Figure 16 represents an overview of the distribution of the raster cells. The most combinations cover only a small area, 117 combinations cover only one raster cell. The largest MPT combination covers 1547 raster cells.

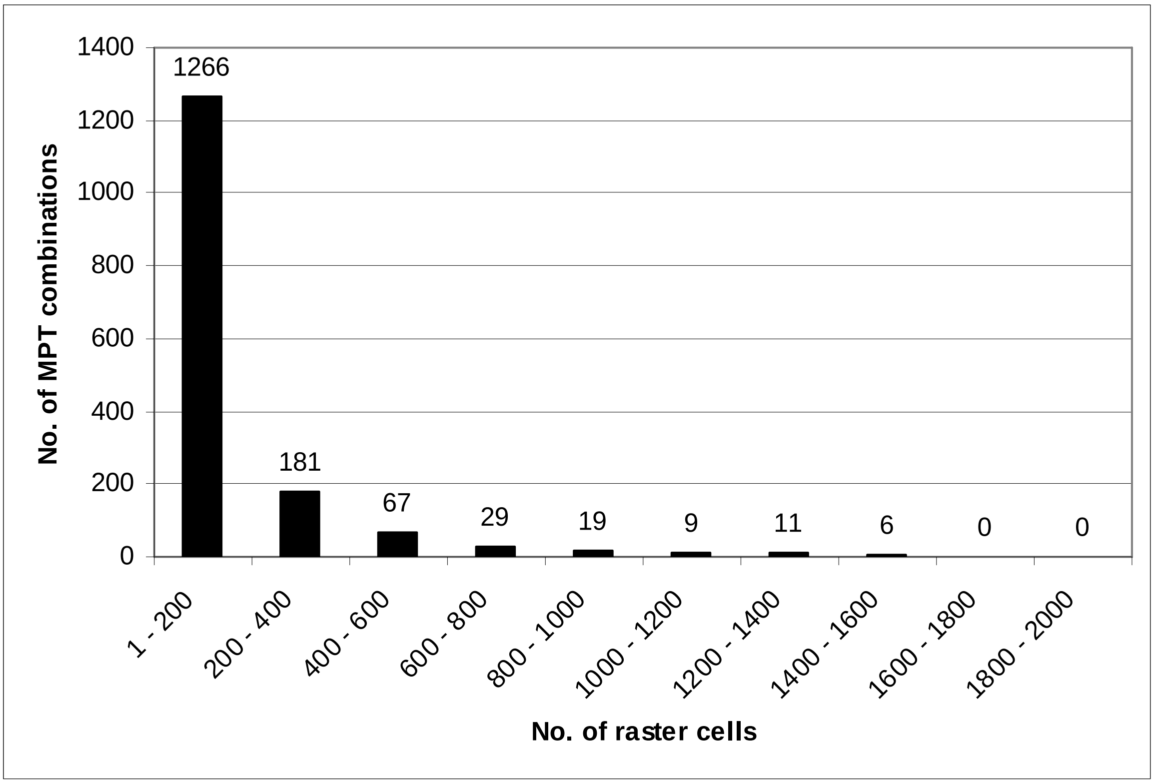


Figure 16: Statistical overview of the MPT combinations

7.4 *Creation of the MPTS combinations*

For the completion of the spatial schematisation, the information for the German soils was allocated to the MPT combinations. For this purpose, the ID of each BÜK soil code was joined to the raster cells. Each raster cell was assigned to the soil code which covers the centre point of the respective cell. The resulting set of combinations was called the MPTS (**M**ARS **P**recipitation **T**emperature **S**oil) combinations. The MPTS data set consists of 7744 unique combinations (UC). Figure 17 represents an overview of the number of cells in each unique combination. The total number of raster cells is 212,480.

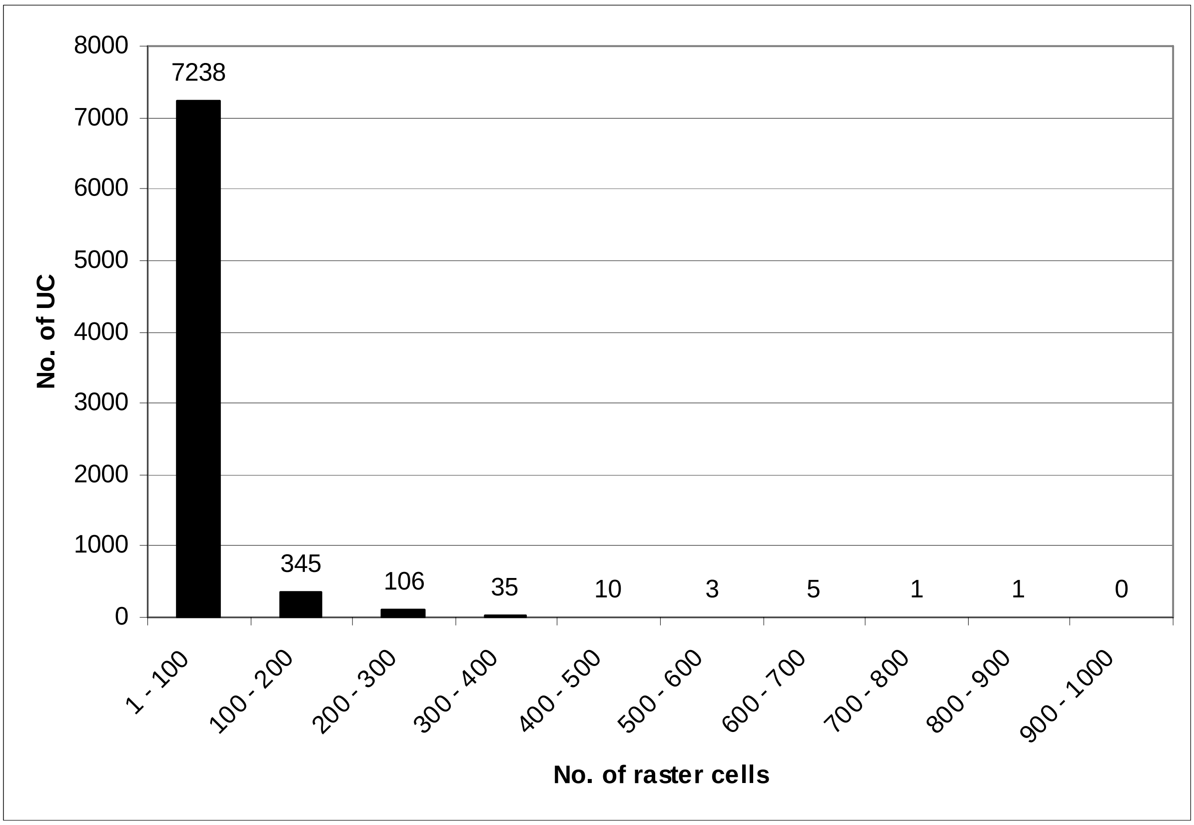


Figure 17: Statistical overview of the unique combinations

The smallest unique combinations are composed of only one raster cell, the largest one of 820 raster cells. Each cell covers an area of 1 km². Thus, the area of the unique combinations ranges between 1 km² and 820 km². Most of the unique combinations are small, only a few are composed of many raster cells.

8 Parameterisation of GeoPEARL_DE

After the derivation of the spatial schematisation, the model input files were set up. GeoPEARL_DE needs several ASCII files for data input and controlling of the calculations. Table 16 lists the files that represent the parameterisation of the spatial schematisation. The first column refers to the file suffix that is used. Nevertheless, all files are ASCII files and can be opened and edited in a text editor. The second column lists the name of the files that were created for the German approach. In some cases, more than one file is required, e.g. the weather files or the crop parameter files. In the following sections, the creation of each file is described.

Table 16: ASCII files for GeoPEARL_DE parameterisation

Suffix	File Name	Description	Remarks
map	Germany_uc.map	**ASCII GRID** • raster value: UC ID	
plo	Germany.plo	**Plot file** • allocates the weather data and the soil data to each UC • includes the relative vulnerability index for reduction of scenarios to be calculated	
unc	Germany.unc	**Crop area database** • lists the total area for each crop per UC	
met	<UC_ID>.met	**Weather file** • lists the daily weather data • one file for each UC available • referenced to the plot file	
sol	Germany.sol	**Soil database** • lists the soil and horizon data • referenced to the plot file	
crp	<name of crop>.crp	**Crop parameters** • lists the parameters for emergence and harvest, plant growth, water uptake and water use for each crop • referenced to the plot file	parameters taken from the FOCUS standard scenario Hamburg
dra	Germany.dra	**Drainage system** • lists the drainage parameters for every UC	no drainage information available for Germany
lbo	Germany.lbo	**Lower boundary condition** • lists the groundwater parameters for every UC	standard value: fixed groundwater level 2 m
mis	crop.mis pastures.mis	**GeoPEARL_DE missers files** • lists the UC to be excluded from calculation when running the model for crops and pastures respectively	

For model simulations, a set of so called control files must be created which gives information on the considered crop, the application scheme, the parameters of the applied substance and the input and output options. These files have to be adapted for each simulation. They are not part of the spatial schematisation which is fixed for all simulations with GeoPEARL_DE. In chapter 8.10, the control files and their function and content are presented. An overview of the output files which represent the results of the model simulations is given in Appendix C.

8.1 The representation of the German spatial schematisation

The map-file represents the spatial schematisation of Germany as an ASCII-GRID. The cell codes show the ID of the unique combination which covers the respective raster cell. The file is not required for the model runs but for the presentation and the analyses of the results. The map-file is the result of the generation of the spatial schematisation which is described in the previous section.

8.2 The representation of the environmental scenarios

8.2.1 Description

In the plo-file, the information for the weather data and the soil data is allocated to each unique combination, i.e. here, the scenarios for the model calculations are defined. The file includes the following information:

- the UC ID
- the area of each unique combination in km²
- the related weather file, corresponds with the number of the met-files
- the soil profile number, corresponds with the content of the file germany.sol
- the crop type
- a correction factor for precipitation (-)
- a correction factor for temperature (°C)
- a correction factor for evapotranspiration (-)
- the irrigation switch (-)
- the maximum ponding depth (m)
- the air boundary layer thickness (m)
- the relative vulnerability rank (see chapter 8.2.2)

The UC ID is referred to the identifier of the unique combinations used in the map-file. Thus the spatial information of the parameterisation files can be joined to the map. Information on all 7744 unique combinations is included. Each unique combination is related to a weather file that is named with the UC ID. For description of the weather files see chapter 8.4. The soil profile number relates the unique combinations to the information of the sol-file (chapter 8.5). Each unique combination is assigned to the soil profile that is relevant for the respective soil code (combination of climate region and soil unit of the BÜK), i.e. the legend unit which covers the raster cells of the unique combination.

The crop type item refers to the crp-file (chapter 8.6). It is a relict of the Dutch approach of GeoPEARL: Here, it was necessary to define a single crop for each scenario (Tiktak et al., 2003). This relation needs to be fixed for calculation definition. In the German schematisation, this constraint is no longer necessary: Each crop parameter set can be assigned to each unique combination. Therefore, a convenient workflow was generated: A standard value “1” was inserted for the crop type item and the crop which should be considered in the simulations is defined in the control files. For further details, see chapter 9.4.

The items “correction factors for precipitation, temperature and evapotranspiration” and “irrigation switch” must not be used for the German parameterisation. Weather corrections are not necessary because a single weather file is available for each scenario. The correction factors should be used if more than one unique combination is related to one weather file and the data of the weather file should be adapted. The items were set to neutral values (“1” for precipitation and evapotranspiration, “0” for temperature). For Germany, no irrigation is assumed and the irrigation switch was set to zero.

The parameter “maximum ponding depth” determines the maximum thickness of the water layer that can be present on the soil profile before surface runoff starts. A standard value of 0.001 m was assumed to intensify runoff from the soil surface (see chapter 9.3.5).

The item “air boundary layer thickness” describes the laminar air boundary layer. The item is required for the calculation of the volatilisation flux of pesticides. A standard value (0.01 m) is chosen for all scenarios according to the Dutch approach.

The index for the relative vulnerability ranking is used for the reduction of the number of the scenarios in a model run (for further details see chapter 8.2.2). The structure of the plo-file is shown in Figure 18.

```
* -------------------------------------------------------------------------------
* SPATIAL SCHEMATISATION FOR GERMANY
* =======================================
*
* File containing the spatial schematisation for Germany.
* Spatial schematisation is based on Bangert (2007)
*
* Version 1 created by Joerg Bangert on 26-Jan-2006
* -------------------------------------------------------------------------------
* Column 1  :  The UC ID
* Column 2  :  Area (km2)
* Column 3  :  Meteo file, corresponds with meteo files in geo file
* Column 4  :  The soil profile number, corresponds with germany.sol, first two digits:
      climate region; last two digits: legend unit from german BUEK 1000
* Column 5  :  The crop type (standard value = 1, don't change!, crops have to be chosen in
      the geo-file by inserting the appropriate crp-file)
* Column 6  :  Correction factor for precipitation (-)
* Column 7  :  Correction temperature (C)
* Column 8  :  Correction factor for evapotranspiration (-)
* Column 9  :  Irrigation switch
* Column 10 :  Maximum ponding depth (m)
* Column 11 :  Air boundary layer thickness (m)
* Column 12 :  Relative vulnerability rank (1 = lowest score; 7672 = highest score)

*    1      2      3    4        5      6      7      8      9     10     11     12

table Plots
     1      2      1  3449       1      1      0      1      0   0.01   0.01      1
     2      6      2  3421       1      1      0      1      0   0.01   0.01      1
(...)
end_table
```

Figure 18: Structure of the plo-file

8.2.2 Implementation of the relative vulnerability index

The relative vulnerability index is used for the reduction of scenarios to be calculated in a GeoPEARL_DE run. Unique combinations that have a similar vulnerability index are summarised to one zone. Then, model calculations are just carried out for a zone. For the reduction of scenarios, GeoPEARL_DE has to be run in a specific mode which is described in detail in Tiktak et al. (2003, 2004a).

The aim of the reduction procedure is to summarise unique combinations by their similarity of vulnerability for pesticide leaching. Similarity was defined by an index. Equal or similar values of the index pinpoint similarity of the leaching behaviour. The index was defined by carrying out multiple GeoPEARL_DE runs considering different application scenarios (i.e. different crops, application dates). Thereby, several leaching concentration values were available for each unique combination. These results were averaged to one single value for each unique combination. The average was used for the derivation of the relative vulnerability index: The scenarios were arranged in ascending order according to the calculated average leaching value. Then, each scenario was assigned a consecutive number beginning with “1” for the scenario with the lowest leaching value. By doing so, unique combinations that show a similar vulnerability index can be summarised to a single zone when setting up a model run. The scenario with the largest area of potential use in the respective zone is taken for the simulations and the result is considered to be valid for the entire zone.

The index depends on the application schedule which was considered during the index generation. Using a single index value for different applications will lead to mismatching of unique combinations to zones for uncommon application schedules. Hence, a set of relative vulnerability indices should be created and the appropriate index should be used for a GeoPEARL_DE run. Because of these conceptual constraints, the relative vulnerability index currently implemented in GeoPEARL_DE is restricted to spring applications to the soil surface for cereals and maize. If other application schedules are requested, a relative vulnerability index appropriate to the requested application schedule should be created or further methods for scenario reduction can be developed.

8.3 The crop database of GeoPEARL_DE

8.3.1 Description

The unc-file represents the crop database of GeoPEARL_DE and lists the total area of the crop for each unique combination. In the file, a row for each scenario and a column for each crop are included. The data in the file are used for scenario selection if the respective option is set in the geo-file (see chapter 8.10.4). Further details are described in Tiktak et al. (2003, 2004a).

In the header of the unc-file, a list of crops is available. GeoPEARL_DE calculations with a focus on relevant cropping area can be carried out using these crops. Additionally, the total agricultural area and the total non-urban area per unique combination are implemented in the table. The total non-urban area is equivalent to the area of the unique combination. The area of the crops and of the total agricultural area derives from the statistical data set provided by the German Federal Statistical Office (2005). The creation of the area values for each scenario is described in the following sections. The structure of the unc-file is shown in Figure 19.

```
* CROP AREA DATABASE FOR GERMANY
* =============================
* File containing the crop area per UC for Germany.
* Input file was generated by Joerg Bangert, March 2006
* The file includes data of the "Federal Statistical Office of Germany" from 2003
* (Federal Statistical Office of Germany (2005): Statistik lokal. CD-ROM.)
* The UC and crop areas are given in (ha)
*-------------------------------------------------------------------------------
table CTB_Crops
1        winter_cereals
2        spring_cereals
3        maize_1
4        maize_2
5        potatoes
6        sugar_beets
7        winter_oil_seed_rape
8        apples
9        vine
10       pastures
11       permanent_crops
12       TotalAgriculturalArea
13       TotalNonUrbanArea
end_table
* maize_1: area calculated by: silage maize + (total_area_cereals - subset_cereals)
* maize_2: area calculated by: silage maize + corn/corn-cob-mix (values given by the
"Statistische Landesämter, 2005")
* winter_oil_seed_rape: includes oil seed rape and other crops called "Handelsgewächse" in the
German statistical data set
* apples: includes fruit trees and berry plantations(derived from the statistical data set and
CORINE land cover)
* vine: includes vineyards (derived from the statistical data set and CORINE land cover)
* permanent_crops: includes orchards, vine and other permanent crops
* for further details see documentation

*record  UC_ID  UC area    1    2    3    4    5    6    7     8    9   10   11    12    13
table PloCrpArea
1  1  200.0  15.2  15.2  22.7  21.9   0.3   0.1   0.5   4.4   4.9   97.6   9.3   155.4   200.0
2  2  600.0   0.1   0.1   1.2   1.2   0.1   0.0   0.1   6.9   0.0  424.9   6.9   433.8   600.0
(...)
end_table
```

Figure 19: Structure of the unc-file

Figure 20 shows the workflow for the creation of the unc-file.

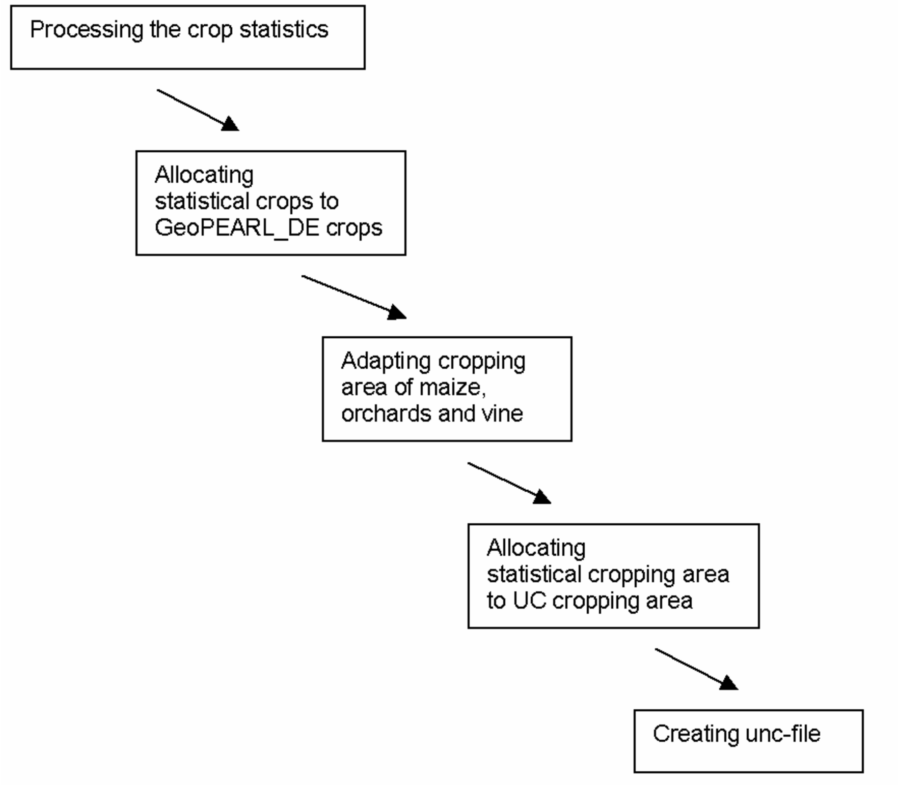


Figure 20: Workflow for creating the unc-file

8.3.2 Allocation of the German crop statistics to GeoPEARL_DE

The information on cropping area is available in the German crop statistics as described in chapter 4.1.5. The pre-processed data (see chapter 5.3) were used for the derivation of the GeoPEARL crop database. Because of the different structure of the official data set and the crop database of GeoPEARL_DE, further pre-processing was necessary: The crops included in the German crop statistics cannot be related one-by-one to the crops used in GeoPEARL_DE because some data are not available in the statistical data set. Table 17 represents an overview of the relation of the crops in the statistical data set and the crops used in GeoPEARL_DE.

Table 17: Allocation of the statistical data to the crops used in GeoPEARL_DE

Crop in GeoPEARL_DE	Allocated statistical data
Winter Cereals, Spring Cereals	Total area of cereals
Maize_1	Area of silage maize + (Area of cereals – Sum of area of all subsets of cereals)
Maize_2	Area of silage maize + Area of corn and corn-cob-mix (derived from an additional data set)
Potatoes	Total area of potatoes
Sugar Beets	Total area of sugar beets
Winter Oil Seed Rape	Total area of industrial crops
Orchards	Total area of permanent crops related to the CLC data set
Vine	Total area of permanent crops related to the CLC data set
Pastures	Total area of pastures
Permanent Crops	Total area of permanent crops
Total Agricultural Area	Total area of agricultural land use

According to FOCUS (2000), all cereals were summarised to the item cereals. The differentiation between winter and spring cereals refers to the crop parameters and the crop management. Differences in the area values do not exist.

8.3.3 Preparation of the final spatial data set

The values of the official data set are related to administrative units whereas GeoPEARL_DE requires data referring to the unique combinations. Therefore, a transformation procedure was carried out which estimates the cultivated area of the unique combinations from the administrative units covering the respective unique combination.

The area of the administrative units (Figure A 2) was reduced to the area representing agricultural land use as defined by the area of interest in GeoPEARL_DE (Figure 9) by intersecting the administrative units data set and the area of interest data set (Figure 21). This data set is used as input for the following rescaling procedure. The area of each object was recalculated. The resulting data set was combined with the data set representing the unique combinations (Figure 22) which represents the output data set of the rescaling procedure. Then, the area of each object was recalculated again. Now, each object in the output data set includes the following information:

- Total area of each crop for each object of the input data set
- Total area of each object in the input data set
- Total area of each object in the output data set

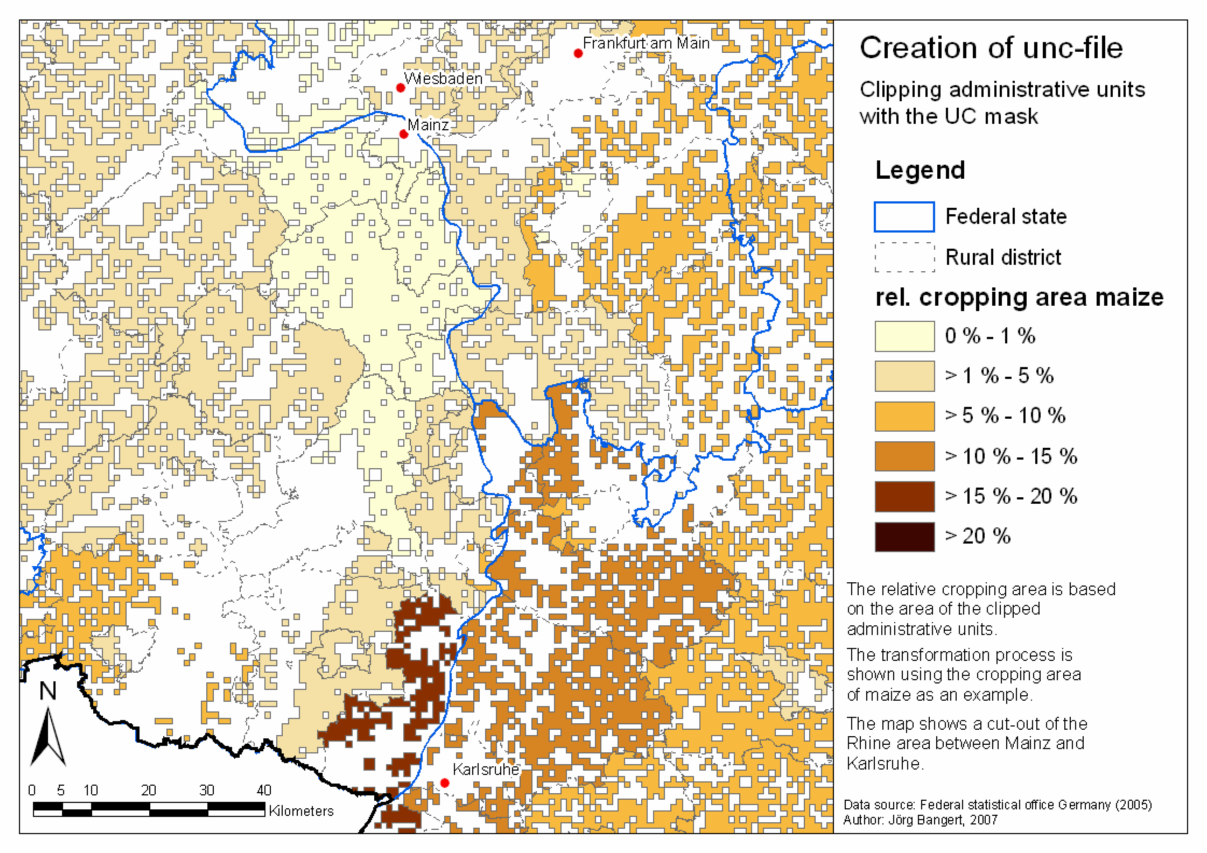
The original agricultural area of the input data set was then rescaled to the polygons of the output data set for each crop using Equation 1:

Equation 1: Recalculation of cropping area

$$A_{io} = A_{ii} * (A_{po}/A_{pi})$$

where A_{io} = Area of crop i in the output data set
A_{ii} = Area of crop i in the input data set
A_{po} = Area of polygon in the output data set
A_{pi} = Area of polygon in the input data set

The output data set was processed to get the original geometry of the spatial schematisation of GeoPEARL_DE (= the unique combinations, see Figure 23) using a dissolving procedure. Thereby, the area of each crop in the output data set is summarised to the total cultivated area for the crop per UC. The information on the cropping area is now present in the data set for all unique combinations. A complete data set including the statistical information of the cropping area related to the unique combinations is available for Germany.



Creation of unc-file

Clipping administrative units with the UC mask

The relative cropping area is based on the area of the clipped administrative units.

The transformation process is shown using the cropping area of maize as an example.

The map shows a cut-out of the Rhine area between Mainz and Karlsruhe.

Data source: Federal statistical office Germany (2005)
Author: Jörg Bangert, 2007

Figure 21: Administrative units reduced to area of interest (cut-out)

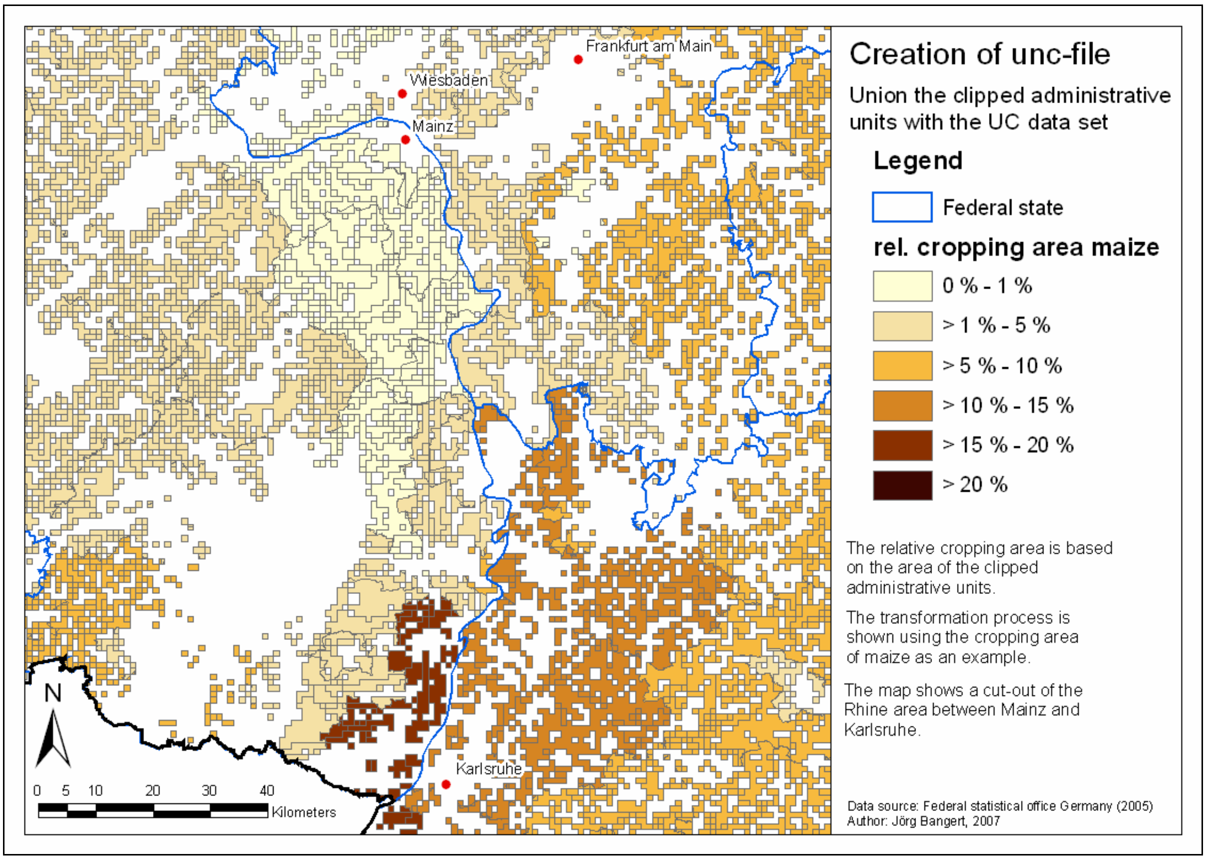


Figure 22: **Combined administrative units with unique combinations (cut-out)**

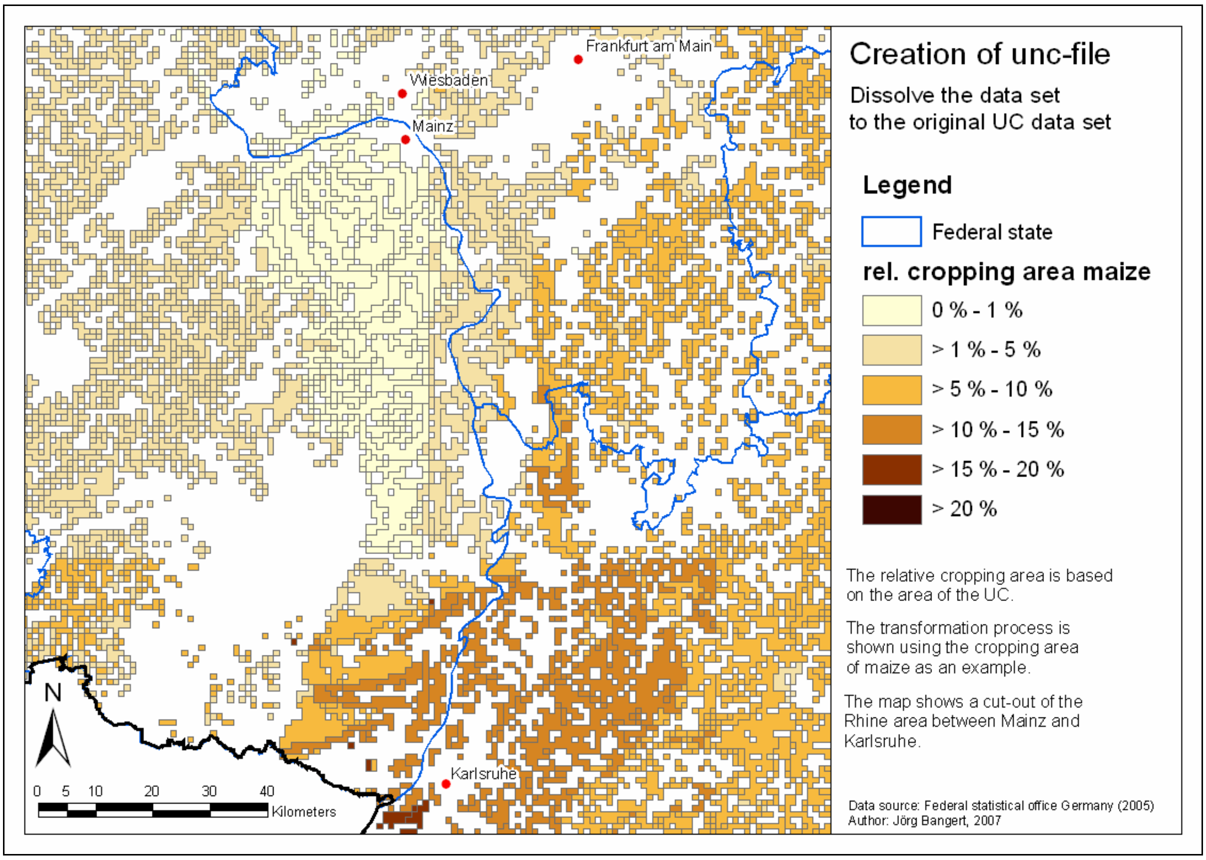


Figure 23: **Result of the dissolving procedure (cut-out)**

8.4 The weather database of GeoPEARL_DE

8.4.1 Description

For GeoPEARL_DE the following weather parameters are required as input:

- Daily minimum of temperature in °C
- Daily maximum of temperature in °C
- Daily precipitation in mm
- Daily potential evapotranspiration from crop canopy in mm

Daily weather parameters are provided by the MARS data set for Europe for 50 km x 50 km tiles (see chapter 4.1.6). This spatial resolution is not sufficient for the purpose of GeoPEARL_DE. Thus, the MARS data were scaled by the DWD data set (see chapter 4.1.7). The DWD data set provides only long-term values for temperature and precipitation but the resolution of 1 km x 1 km is appropriate to the scale of GeoPEARL_DE. The aim of this section is to describe the procedure of scaling the daily weather data of MARS using the DWD data to get a new weather data set with high spatial as well as high temporal resolution. This results in a single weather scenario for each unique combination which is stored in a met-file. The met-files were named by the related UC ID to simplify their association. In the DWD data set, no data on the potential evapotranspiration is provided. Thus, the MARS data can not be scaled for this item and the evapotranspiration value of the covering MARS tile was assigned to each UC. For GeoPEARL_DE, the MARS data of the years 1992 to 2004 are available. Thus in GeoPEARL_DE, calculations for 13 years can be carried out. The long-term values of the DWD data were measured in the time period from 1961 to 1990.

Figure 24 shows the header of a met-file. The items “radiation”, “humidity”, and “wind speed” are flagged to “no data” value (-99) as calculations are based on evapotranspiration.

```
*-------------------------------------------------------------------------
* Meteofiles for GeoPEARL
*
* Station DD   MM   YYYY     RAD   Tmin   Tmax   HUM  WIND    RAIN   ETref
*         nr   nr     nr   kJ/m2      C      C   kPa   m/s      mm      mm
*-------------------------------------------------------------------------
  7744     1    1   1901     294  -0.89   5.21   -99   -99       0    0.41
  7744     2    1   1901       0   4.61   6.11   -99   -99       0    1.51
  7744     3    1   1901       0   5.51   6.51   -99   -99       0    2.52
(…)
  7744    31   12   1945    1062   4.01   5.81   -99   -99   7.455       0
```

Figure 24: Structure of a met-file

Figure 25 shows the workflow for the creation of the met-files.

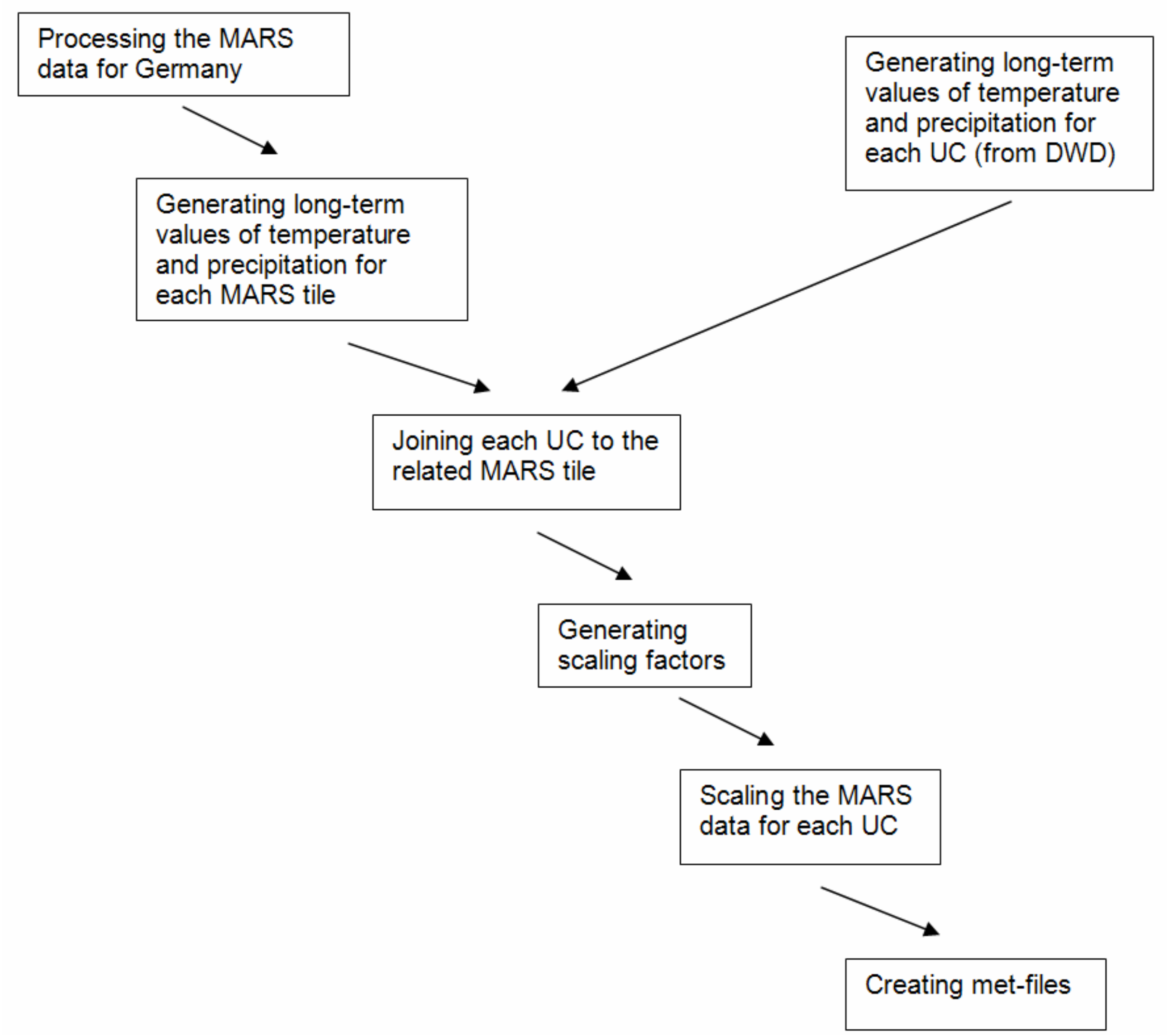


Figure 25: Workflow for creating the met-files

8.4.2 Preparation of the MARS data

The original MARS data are stored in txt-files. For each year (1992 – 2004), one txt-file is available containing the data for all MARS tiles. The data were processed to obtain monthly long-term values for temperature and precipitation which were derived from the daily data and the time period was transformed from 1992 – 2004 to 1901 – 1913 according to FOCUS (2000). This step was necessary to avoid code problems in the software with the change of the millennium from 1999 to 2000. Nevertheless, the data represent current climate parameters.

According to FOCUS (2000), GeoPEARL_DE requires a “warming up” period of six years for calibration of the system. During this period, the soil moisture and substance concentrations will level off. Therefore, the first six years (1992 – 1997) were duplicated and set at the beginning of the data set. If the considered substance is applied every two years or even every three years, the calculation years have to be duplicated or triplicated, respectively. Thus, the time period included in the 186 Excel files was extended. The 13 original years were triplicated and set to the end of the data set. Now the data set includes daily weather data for 45 years. Finally, the leap days were adapted. A similar procedure was set up for the derivation of the FOCUS groundwater scenarios as described in FOCUS (2000).

8.4.3 Preparation of the DWD data

The DWD data set includes long-term monthly values for temperature and precipitation for a 1 km x 1 km raster of Germany. The data were transformed to average values for each unique combination with the help of a ZONAL function in the GIS. Average values for each of the 24 DWD data sets (12 for temperature and 12 for precipitation) were calculated for each unique combination.

8.4.4 Derivation of the scaling factors and of the weather database

After the preparation of the MARS data (see chapter 8.4.2) and the DWD data (see chapter 8.4.3), the basis for the derivation of the scaling factors was set up. Each unique combination was allocated to the MARS tile that covers the respective unique combinations. Thereby, the calculated average climate values from the MARS data set and the DWD data set can be joined together. Then the calculation of the scaling factors for the temperature was performed by Equation 2:

Equation 2: Calculation of the scaling factor for temperature

Factor (T) = Monthly Mean Temperature UC – Monthly Mean Temperature MARS

The calculation of the scaling factors for the precipitation was performed by Equation 3:

Equation 3: Calculation of the scaling factor for precipitation

Factor (P) = Monthly Sum Precipitation UC / Monthly Sum Precipitation MARS

For each month and each unique combination, a single scaling factor for temperature and precipitation was now available. The scaling factor for the temperature was added to the respective MARS daily temperature value and the MARS values of precipitation were multiplied by the scaling factor. The resulting weather data were stored as space separated text files with the suffix “met”. A similar method for the derivation of the weather data is used for the development of EuroPEARL as described in Tiktak et al. (2004b).

Statistical tests were carried out in order to investigate if the scaling procedure shows appropriate results. A description is available in Appendix B. The result of the test shows that the weather data becomes wetter and colder in average compared with the original MARS data.

8.5 The soil database of GeoPEARL_DE

8.5.1 Description

In the sol-file, the soil database of GeoPEARL_DE is stored. The file includes soil-related parameters for all soil profiles and the horizon-related parameters for each soil profile. The soil profiles are referred to the plo-file (chapter 8.2.1). The first part of the sol-file lists the parameters that are valid for all profiles. In this section, the information on soil evaporation, the relative diffusion coefficient, the depth dependence of transformation and the depth dependence of sorption are available.

In the second section of the file, the horizon-related parameters are listed. The following parameters have to be specified for each horizon:

- Soil profile number
- Soil horizon number
- Horizon thickness (m)
- Number of numerical soil compartments
- Sand fraction (kg kg^{-1}) as part of mineral soil
- Silt fraction (kg kg^{-1}) as part of mineral soil
- Clay fraction (kg kg^{-1}) as part of mineral soil
- Organic matter content (kg kg^{-1})
- pH (required for calculations of substances with pH-dependent sorption behaviour, for GeoPEARL_DE, the pH-CaCl$_2$-value is used)
- Saturated soil water content (m^3 m^{-3})
- Residual water content (m^3 m^{-3})
- Parameter alpha (dry) (cm^{-1})
- Parameter alpha (wet) (cm^{-1})
- Parameter N (-)
- Saturated hydraulic conductivity (m d^{-1})
- Physical saturated hydraulic conductivity (m d^{-1})
- Parameter L (-)
- Dispersion length (m)
- Sesqui-oxide content (mmol kg^{-1}) (required for calculations of substances with sesqui-oxide dependent leaching behaviour)

Figure 26 shows the structure of the sol-file.

```
*     ------------------------------------------------------------------------------
*     SOIL DATABASE FOR Germany
*     ========================================
*     File containing the soil database for Germany.
*     The first part of the file contains parameters that are assumed to be spatially
*     constant. The second part of the file contains the spatially distributed
*     parameters.
*
*     ------------------------------------------------------------------------------
*     Soil evaporation

Black OptSolEvp                  Use the Black option for soil evaporation
0.005 PrcMinEvp         (m.d-1)  Minimum rainfall to reset Black model
0.79  CofRedEvp         (cm1/2)  Reduction parameter in Black equation
1     FacEvpSol         (-)      Crop factor for soil evaporation

*     ------------------------------------------------------------------------------
*     Dispersion length and relative diffusion coefficient
*     GeoPEARL only supports the Millington Quirk option!

2.00  ExpDifLiqMilNom   (-)      Exponent in nominator of equation [0.1|5]
0.67  ExpDifLiqMilDen   (-)      Exponent in denominator of eqn    [0.1|2]
2.00  ExpDifGasMilNom   (-)      Exponent in nominator of equation [0.1|5]
0.67  ExpDifGasMilDen   (-)      Exponent in denominator of eqn    [0.1|2]

*     ------------------------------------------------------------------------------
*     Depth dependence of transformation
table FacZTra (-)
0.00  1.00
0.30  1.00
0.31  0.50
0.60  0.50
0.61  0.30
1.00  0.30
1.01  0.00
50.00 0.00
end_table

*     ------------------------------------------------------------------------------
*     Depth dependence of sorption
table FacZSor (-)
0.00  1.00
0.30  1.00
0.31  1.00
0.60  1.00
0.61  1.00
1.00  1.00
1.01  1.00
50.00 1.00
end_table

*     ------------------------------------------------------------------------------
*     Column 1  :  Soil profile number
*     Column 2  :  Soil horizon number
*     Column 3  :  Horizon thickness (m)
*     Column 4  :  Number of numerical soil compartments
*     Column 5  :  Sand fraction (kg.kg-1) as part of mineral soil
*     Column 6  :  Silt fraction (kg.kg-1) as part of mineral soil
*     Column 7  :  Clay fraction (kg.kg-1) as part of mineral soil
*     Column 8  :  Organic matter content (kg.kg-1)
*     Column 9  :  pH-CaCl2
*     Column 10 :  Saturated soil water content (m3.m-3)
*     Column 11 :  Residual water content (m3.m-3)
*     Column 12 :  Parameter alpha (dry) (cm-1)
*     Column 13 :  Parameter alpha (wet) (cm-1)
*     Column 14 :  Parameter n (-)
*     Column 15 :  Saturated hydraulic conductivity (m.d-1)
*     Column 16 :  Physical saturated hydraulic conductivity (m.d-1)
*     Column 17 :  Parameter L (-)
*     Column 18 :  Dispersion length (m)
*     Column 19 :  Sesqui-oxide content (mmol.kg-1)

*---------------------------------------------------------------
table SoilProfiles
3301  1   0.3  12  0.929  0.04   0.025  0.03   5.5  0.363  0.01  0.058  0.058  1.5   0.9877  0.9877  -0.65
0.05  0
3301  2  0.05   1  0.929  0.046  0.025  0.03   5.5  0.363  0.01  0.058  0.058  1.5   0.9877  0.9877  -0.65
0.05  0
3301  3  0.15   3  0.929  0.046  0.025  0.005  5.5  0.368  0.01  0.066  0.066  1.61  1.6674  1.6674   0.53
0.05  0
(…)
end_table
```

Figure 26: Structure of the sol-file

Figure 27 shows the workflow for the creation of the sol-file.

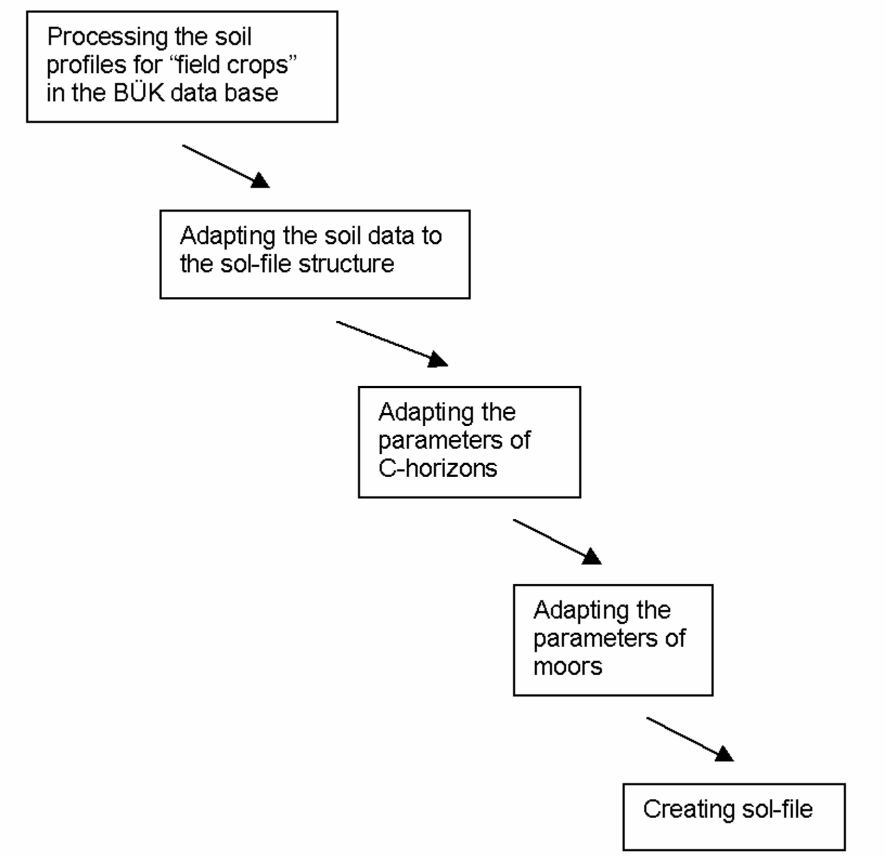


Figure 27: **Workflow for creating the sol-file**

8.5.2 Preparation of the soil data

The data required for the sol-file were taken from the German soil database BÜK 1000 (BGR, 2005). As described in chapter 5.5, for each BÜK combination of climate region and soil unit, the provided soil profile for agricultural land use was used. Most of the required parameters are available in the database. The van Genuchten parameters for description of the soil water flow were provided in an addendum to the BÜK 1000 by the BGR (BGR, 2006). The thickness of the soil profile was set to 3 m for each soil profile in order to avoid calculation problems regarding the groundwater table at 2 m (see chapter 8.8). Thus, many soil profiles were extended to 3 m by stretching the last horizon.

Soil profile number

The soil profile number is equivalent to the soil code of the BÜK data set used for the spatial schematisation (chapter 5.5). It represents a combination of the climate region and the soil legend unit.

Soil horizon number

The soil horizon number is a consecutive number starting with “1” for each soil profile. The soil profiles must have horizon boundaries at 30 cm, 60 cm, 100 cm and 200 cm in order to relate the values of the depth dependence of transformation and the number of numerical compartments (see below). When the original soil profiles were not split at these depths, a new boundary was introduced. The resulting horizons offer the same properties as the parent horizon. The difference between them is the different factor for transformation and a different layer thickness of the soil compartments. Thus, the number of horizons increases in most cases compared to the original data set.

Horizon thickness (m)

The parameter “horizon thickness” was derived from the data of the upper and lower horizon boundaries in the BÜK. The thickness was adapted when introducing a new horizon.

Number of numerical soil compartments

GeoPEARL divides the soil horizons into a user-defined number of layers for the simulations – the soil compartments. The greater the number of the layers used, the higher is the accuracy and the longer is the computation time. As a compromise, the number of numerical compartments was defined by the following rules according to FOCUS PEARL (FOCUS, 2000):

- 0 cm – 30 cm: layer-thickness 2.5 cm
- 30 cm – 200 cm: layer-thickness 5 cm
- 200 cm – 300 cm: layer-thickness 10 cm

Sand/Silt/Clay fraction (kg kg^{-1}) as part of mineral soil

In the BÜK database, the soil texture is available as classified data according to the German guidance for soil mapping (AG Boden, 1994). For GeoPEARL_DE, numerical values are required. Thus, the BÜK data were changed to numerical values using the centre of each class for the soil fractions according to BGR (2006) (see Table 18).

Table 18: Translation of the classified soil texture

Texture code	Clay (%)	Silt (%)	Sand (%)
fSms	2.5	5	92.5
Hh	6.5	17.5	76
Hn	6.5	17.5	76
Ls2	21	45	34
Ls3	21	35	44
Ls4	21	22.5	56.5
Lt2	30	40	30
Lt3	40	40	20
Lts	35	22.5	42.5
Lu	23.5	57.5	19
mSfs	2.5	5	92.5
Sl2	6.5	17.5	76
Sl3	10	25	65
Sl4	14.5	25	60.5
Slu	12.5	45	42.5
Ss	2.5	5	92.5
St2	11	5	84
St3	21	7.5	71.5
Su2	2.5	17.5	80
Su3	4	32.5	63.5
Su4	4	45	51
Tl	55	22.5	22.5
Ts2	55	7.5	37.5
Ts3	40	7.5	52.5
Ts4	30	7.5	62.5
Tt	82.5	0	17.5
Tu2	55	32.5	12.5
Tu3	37.5	52.5	10
Tu4	30	65	5
Uls	12.5	57.5	30
Us	4	65	31
Ut2	10	76.5	13.5
Ut3	14.5	74	11.5
Ut4	21	70	9
Uu	4	86	10

The break value of the soil texture classes “sand” and “silt” in the BÜK is different from the required international value. Thus, the content of sand and silt was transformed to the international system using a log-linear recalculation of the break value according to BGR (2006).

Organic matter content (kg kg^{-1})

The organic matter (OM) content in the BÜK data set was represented as classified data according to AG Boden (1994). According to BGR (2006), the classified data were changed to numerical values using the centre of the class boundaries (see Table 19). For some soil horizons – C-horizons in all cases – the organic matter content was not available. The respective value was set to “0”.

Table 19: Translation of the classified organic matter content

OM class	OM content (kg kg^{-1})
h0	0
h1	0.005
h2	0.015
h3	0.03
h4	0.06
h5	0.115
h6	0.225
h7	0.3

pH-value

In the BÜK data set, the pH-value was available as classified data according to AG Boden (1994). The classified data were transformed to numerical values using the centre of the class boundaries (see Table 20). GeoPEARL_DE requires pH-values for simulations with substances having a pH-dependent sorption behaviour.

Table 20: Translation of the classified pH-values

pH class	pH-value
-99	-99
a0	7
a0/s0	7
a1	7.25
a2	7.75
a3	8.5
a4	9.5
a5	10.5
a6	12
s0	7
s1	6.75
s2	6.25
s3	5.5
s4	4.5
s5	3.5
s6	2

Van Genuchten parameters – soil water flow

GeoPEARL_DE requires the following parameters for estimation of the soil water flow:

- Saturated soil water content (m^3 m^{-3})
- Residual water content (m^3 m^{-3})
- Parameter alpha (dry) (cm^{-1})
- Parameter alpha (wet) (cm^{-1})
- Parameter n (-)
- Saturated hydraulic conductivity (m d^{-1})
- Physical saturated hydraulic conductivity (m d^{-1})
- Parameter L (-)

Normally, van Genuchten parameters are not measured during field experiments. Thus, methods were developed to estimate the soil water flow parameters from other soil related parameters. The BGR used a method provided in the HYPRES project (Wösten, 1998, 1999) for parameter estimation. The method uses the content of clay, silt, and sand, the bulk density, the organic matter content, and an index for layer depth for the estimation of the van Genuchten parameters. The values are provided in BGR (2006) for the profiles with land use “field crops”.

The parameters for alpha wet and alpha dry and for the saturated hydraulic conductivity and the physical saturated hydraulic conductivity, respectively, were assumed to be equal according the Dutch approach of GeoPEARL. For the BÜK soil units 6 and 7 (moors) and for the C-horizons of the soil profiles, no van Genuchten parameters are available because of missing parameters for estimation (see BGR, 2006). Thus, for these profiles, realistic worst-case scenarios were developed (chapter 8.5.3 and chapter 8.5.4) and the missing van Genuchten parameters were derived according to the method used in BGR (2006).

Dispersion length (m)

The parameter of the dispersion length influences the transport of a substance in the liquid phase of the soil together with other parameters. A standard value of 0.05 m was used according to the PEARL guideline (Tiktak et al., 2000).

Sesqui-oxide content (mmol kg^{-1})

In the BÜK data set, no information on the sesqui-oxide content of the soil horizons is available. The parameter was set to “0” as a standard value. This setting allows no calculation of substances with sesqui-oxide dependent leaching behaviour which is a very uncommon case.

8.5.3 Parameterisation of the C-horizons

Soil profiles must have a depth of at least the evaluation depth that is set to 1 m according to FOCUS (2000). The groundwater table was assumed to be at 2 m below ground for Germany as a standard (see chapter 8.8). For technical reasons, the soil profiles should be deeper than the groundwater table to avoid problems with the calculation of the water flux. Thus, it was proposed to extend all profiles up to 300 cm. Some profiles in the BÜK database end at 50 cm, then the C-horizon without parameters follows. However, for model calculations, parameters for all horizons are required. Thus, the C-horizons were parameterised as follows:

- Soil texture: pure sand
- Organic matter: 0 %
- van Genuchten parameters: tabulated values from HYPRES database (Wösten, 1998).
- pH-value: -99 (no data)

Tests were carried out to evaluate the presented parameterisation. The described approach represents a worst-case scenario regarding the leaching of substances to the groundwater.

8.5.4 Parameterisation of the moors

In the BÜK 1000, the soil units 6 and 7 represent moors. For one climate region, a realistic soil profile for agricultural land use is available: soil unit 6, climate region 34. For the other climate regions, the related profiles for agricultural land use do not represent profiles that can be used for cropping regarding the pH-value (pH 4.5) and the soil texture. The profiles represent moor profiles with very high OM content that cannot be used for parameterisation because of the missing values for the soil texture. For these legend units, realistic soil profiles for agricultural land use on former moors were defined. A realistic worst-case scenario was assumed to make sure that the leaching behaviour is not underestimated.

The H-horizons of the moor profiles were parameterised as follows:

- **Soil texture**: The values from the last horizon (which is in all cases a mineral horizon) were taken.
- **Organic matter content**: For the first horizon a value of 11.5 % was set, for the other horizons a value of 6 %.
- **pH-value**: The pH-value of each horizon was increased by one class (German pH-classification, AG Boden, 1994).
- **Van Genuchten parameters** were derived using the HYPRES method (Wösten, 1998, 1999).
- **Bulk density** (required for the derivation of the van Genuchten parameters): The value was set to 1.15 g cm^{-3}.
- **Top soil indicator** (required for the derivation of the van Genuchten parameters): The Hp-horizon was considered as top soil, the other horizons as subsoil.

The parameterisation was carried out using the following assumptions:

- It can be assumed that the subsoil material was used for melioration of the moors. This finding is consistent with information from literature (AG Boden, 2005; Zeitz, 2006 pers. comm.; NLfB, 1997). Therefore, the subsoil material was set as texture of the mineral top soil.
- In the literature, the profiles of cultivated moors show an organic matter content of h5 (NLfB, 1997) and h4 (Frielinghaus et al., 2003).
- pH-value: The pH-values of cultivated moors show a range from ca. pH 4.5 (NLfB, 1997) to pH 7.5 (Frielinghaus et al., 2003). The BÜK soil unit 3406 shows pH 7 – 6.75. The original moor profiles in the BÜK show pH 4.5. This value was assumed to be too acid and the values were increased by one class to pH 5.5.
- Bulk density: The value was derived from values described in the literature (Frielinghaus et al., 2003).

8.6 The crop parameter database of GeoPEARL_DE

In the crp-file the properties of the simulated crops are defined. The following parameters are required:

- Crop calendar
    - Emergence date
    - Harvest date
- Crop parameters related to crop development stage
    - Leaf area index
    - Crop factor
    - Rooting depth
    - Crop height
- Root density
- Crop water use
    - Anaerobiosis point
    - Wet reduction point
    - Dry reduction point
    - Wilting point
    - Minimum canopy resistance
    - Extinction coefficients for solar radiation
    - Constant in Braden equation for interception

For each crop for which calculations shall be carried out, a crp-file is required. Currently, in GeoPEARL_DE, a parameterisation for the following crops is available:

- Spring cereals
- Winter cereals
- Grass
- Maize
- Winter oil seed rape
- Peas
- Potatoes
- Sugar beets
- Apples
- Vine
- Pastures

The crop parameters of the FOCUS Hamburg scenario (FOCUS, 2000) were chosen for the parameterisation. They are equal for all GeoPEARL_DE scenarios. It is assumed that there are no spatial differences regarding the different regions in Germany. If it will be necessary to use spatially differentiated crop parameters in future, they can be inserted into the crp-file of the respective crop. Then, in the plo-file, the unique combinations can be related to the respective parameter set by specifying the crop type item (see chapter 10.1). Figure 28 shows an example of a crop file (winter cereals).

```
* CROP PARAMETER DATABASE WINTER CEREALS FOR Germany
* ==================================================
* File containing the crop parameters 'winter cereals' for Germany.
* The Crop Calendar and the data of the development stages
* are taken from the standard Hamburg scenario from FOCUS
* PEARL 2.2.2.
* Version 1 created by Joerg Bangert in 2006
* ,,> Compatible with GeoPEARL version 1.4.1.
*-------------------------------------------------------------------------------
* Relationship between crop name and the crop number in the plot file
table SwapCrops
1  wcereals
end_table
*-------------------------------------------------------------------------------
* Parameters that apply to all crops
Yes             RepeatCrops         Repeat the crop calendars (Yes/No)?
Fixed           OptLenCrp           Development stage fixed or variable?
*-------------------------------------------------------------------------------
* Crop 1: Winter Cereals
[wcereals]

wcereals             CropCalendar

* Emergence and harvest date of crop.
* Note: Length of growing season must be constant for one crop
* If repeat crops: Specification of year not required
table  Crops
01-Nov    10-Aug  wcereals
end_table

* Crop parameters as a function of development stage
* Column 1: Development stage: 0 = emergence; 1 = harvest (-)           [0|1]
* Column 2: LAI: Leaf Area Index                          (m2.m-2)      [0|12]
* Column 3: FacCrp: Crop factor                           (-)           [0.5|1.5]
* Column 4: ZRoot: Rooting depth                          (m)           [0|10]
* Column 5: HeightCrp:  Crop height                       (m)           [0|10]
table  CrpPar_wcereals
0      0.0    1.00    0.0    0
0.655  0.1    1.00    0.2    0
0.755  3.8    0.74    1.1    0
1      3.8    0.74    1.1    0
end_table

* Root density table (first column is relative depth)
* Column 1: Relative depth 0 = soil surface; 1 = DepRoot  (-)           [0|1]
* Column 2: Root density distribution                     (-)           [0|1]
table  RootDensity_wcereals
0      1
1      1
end_table

* Crop water use
0.0          HLim1_wcereals     (cm)        Anaerobiosis point  [-100|0]
-1.0         HLim2_wcereals     (cm)        Wet reduction point [-1000|0]
-500.0       HLim3U_wcereals    (cm)        Dry reduction point [-10000|0]
-900.0       HLim3L_wcereals    (cm)        Dry reduction point [-10000|0]
-16000.0     HLim4_wcereals     (cm)        Wilting point       [-16000|0]

70.0        RstEvpCrp_wcereals (s.m-1)     Min. canopy resistance [0|1000]
0.39        CofExtDif_wcereals (-)         Extinction coef. for solar radiation [0|2]
1.00        CofExtDir_wcereals (-)         Extinction coef. for solar radiation [0|2]
0.0001      CofIntCrp_wcereals (cm)        Constant in Braden eq for interception [0|1]

* Automatic irrigation options
0.2      ZTensiometer_wcereals (m)    Depth of (virtual) tensiometer [0|10]
-100.0   PreHeaIrrSta_wcereals (cm)   Critical pressure head for irrigation [-1e6|-100]

* If OptLenCrp = Variable:
0.0          TemSumSta_wcereals     (C)     Start value of temperature sum [-10|20]
1050.0       TemSumEmgAnt_wcereals  (C)     Sum from emergence to anthesis [0|1e4]
1000.0       TemSumAntMat_wcereals  (C)     Sum from anthesis to maturity  [0|1e4]

[end_wcereals]
```

Figure 28: Structure of a crp-file

8.7 The drainage database of GeoPEARL_DE

In the dra-file, the drainage system for each scenario is specified. As no spatial information on drainage is available for Germany, the respective model routines were switched of by setting the option of lateral drainage and surface drainage to “No”. No further entry needs to be made in the table. Nevertheless, the dra-file must be present in GeoPEARL_DE. If in the future, appropriate drainage data becomes available, the dra-file can be parameterised to implement this information in the application. Figure 29 shows the structure of the dra-file.

```
*    -------------------------------------------------------------------------------
*    DRAINAGE SYSTEM OF Germany
*    ==========================================
*
*    There are no parameters of the drainage systems in Germany available.
*    The 'OptDra' and the 'OptSurDra' options were set to 'No', so that
*    no drainage is calculated.
*    You don't have to change these options.
*
*    Version 1 created by Joerg Bangert March 2006
*    ,,> Compatible with GeoPEARL version 1.4.1.
*    -------------------------------------------------------------------------------

*    -------------------------------------------------------------------------------
*    General control options for drainage module
No   OptDra           Lateral drainage? (No|Extended|Basic)
No   OptSurDra        Simulate surface drainage?

*    -------------------------------------------------------------------------------
*    Width of draiange system
2.5  WidthPrimary     (m)     Width of primary drain system
1.5  WidthSecondary   (m)     Width of secondary drain system
0.5  WidthTertiary    (m)     Width of tertiary drain system
0.1  WidthTubes       (m)     Width of tube drain system
0.1  WidthSurfaceDrain(m)     Width of surface drain system

*    -------------------------------------------------------------------------------
*    Characteristics of the surface drainage system
30   RstSurDraDeep    (d)     Resistance of surface drain system
30   RstSurDraShallow (d)     Resistance of surface drain system

*    -------------------------------------------------------------------------------
*    Column 1  :  The plot ID
*    Column 2  :  Distance between primary drainage system (m)
*    Column 3  :  Depth of bottom of primary drainage system (m)
*    Column 4  :  Surface water level in primary drainage system (m)
*    Column 5  :  Drainage resistance of primary drainage system (d)
*    Column 6  :  Infiltration resistance of primary drainage system (d)
*    Column 7  :  Distance between secondary drainage system (m)
*    Column 8  :  Depth of bottom of secondary drainage system (m)
*    Column 9  :  Surface water level in secondary drainage system (m)
*    Column 10 :  Drainage resistance of secondary drainage system (d)
*    Column 11 :  Infiltration resistance of secondary drainage system (d)
*    Column 12 :  Distance between tertiary drainage system (m)
*    Column 13 :  Depth of bottom of tertiary drainage system (m)
*    Column 14 :  Surface water level in tertiary drainage system (m)
*    Column 15 :  Drainage resistance of tertiary drainage system (d)
*    Column 16 :  Infiltration resistance of tertiary drainage system (d)
*    Column 17 :  Distance between pipe drainage system (m)
*    Column 18 :  Depth of bottom of pipe drainage system (m)
*    Column 19 :  Surface water level in pipe drainage system (m)
*    Column 20 :  Drainage resistance of pipe drainage system (d)
*    Column 21 :  Infiltration resistance of pipe drainage system (d)
*    Column 22 :  Surface water level in summer (m)
*    Column 23 :  Surface water level in winter (m)
*    Column 24 :  Surface water supply capacity

table Drainage
end_table
```

Figure 29: Structure of the dra-file

8.8 The groundwater database of GeoPEARL_DE

In the lbo-file, the lower boundary conditions for each unique combination are described. No spatial information on groundwater depth was available at the scale of interest for the GeoPEARL_DE approach. Thus, a constant type of lower boundary condition was assumed, i.e. a groundwater level of 2 m below ground according to the assumptions made for EuroPEARL (see Tiktak et al., 2004b). Figure 30 shows the structure of the lbo-file.

```
* -------------------------------------------------------------------------------
*  LOWER BOUNDARY CONDITIONS FOR Germany
*  =====================================================
*
*  File containing the regional groundwater system for Germany
*  As there are no parameters only the first 'option OptLbo = GrwLev'
*  is used.
*
*  Version 1 created by Joerg Bangert March 2006
*  ,,> Compatible with GeoPEARL version 1.4.1
* -------------------------------------------------------------------------------

* -------------------------------------------------------------------------------
*  Type of boundary condition
  GrwLev    OptLbo      GrwLev, Flux, Cauchy, Freedrain, Mixed
  No        Transient   Transient coupling with regional model?

* -------------------------------------------------------------------------------
*  Maximum seepage flux
  -1.2      QBotAveMax   (mm.d-1) Maximum seepage flux

* -------------------------------------------------------------------------------
*  GroundwaterSystem table. Format depends on OptLbo
*
*  If OptLbo = GrwLev
*  Column 1  :  The plot ID
*  Column 2  :  Groundwater level
*
*  If OptLbo = Flux
*  Column 1  :  The plot ID
*  Column 2  :  Initial groundwater level
*  Column 3  :  Average flux at the lower boundary (mm.d-1)
*  Column 4  :  Amplitude of the lower boundary flux (mm.d-1)
*  Column 5  :  Day that the maximum flux is reached
*
*  If OptLbo = Cauchy
*  Column 1  :  The plot ID
*  Column 2  :  Initial groundwater level (m)
*  Column 3  :  Resistance of aquitard (d)
*  Column 4  :  Head below aquitard (m)
*
*  If OptLbo = Mixed
*  Column 1  :  The plot ID
*  Column 2  :  Initial groundwater level (m)
*  Column 3  :  Regional flux at the lower boundary (mm.d-1)
*  Column 4  :  Resistance of aquitard (d)
*  Column 5  :  Head below aquitard (m)
*
*         1           2         3         4         5         6
table GroundwaterSystem
          1          -2         0         0         0         0
(…)
       7744          -2         0         0         0         0
end_table
```

Figure 30: Structure of the lbo-file

8.9 The list of unique combinations excluded from model calculations

The mis-files list the unique combinations that are excluded from model calculations. They contain the scenarios for soil profiles with agricultural land use that are not provided in the BÜK database (see chapter 5.5). The file “pastures.mis” contains the UC ID’s for land use field crops as well as pastures for which no soil profiles are available. These scenarios have to be excluded from any model calculation. In the file “crop.mis” the UC ID’s are included for those combinations that cannot be parameterised with soil profiles related to field crops but can be parameterised for pastures. These scenarios can be used for model calculations of pastures but not for calculations considering field crops. Figure 31 shows the structure of a mis-file.

```
*------------------------------------------------------------------------------
* MISSERS FOR Germany
* ============================
*
* File containing the UC for combinations for which no soil profiles with land use "crop" are
available.
* The file has to be used for GeoPearl runs with crops.
* This file is generated by Joerg Bangert
*
*
*------------------------------------------------------------------------------

table SwapMissers
1       3
2       4
3       5
(…)
72      6127
end_table
```

Figure 31: Structure of a mis-file

8.10 Control file parameterisation

The control files are necessary for the set-up of a simulation run. Each simulation needs a new adaptation of the control files for the respective purposes. The files are not part of the spatial schematisation and their functions were not changed in this project. Therefore, this document does not give a detailed manual of the set up of the control files. The user is referred to the GeoPEARL manual as described in Tiktak et al. (2003, 2004a). Nevertheless, the required files are shortly presented here and their function is described. The following files are necessary for model runs:

- the app-file (including the application schemes)
- the cmp-file (including the substance parameters)
- the lis-file (optional, including the scenarios to be calculated)
- the geo-file (including the control parameters)
- the ctr-file (including the output options)

8.10.1 The application scheme

In the app-file, the application schemes for the scenarios are specified. The application scheme comprehends the following information:

- Application frequency
- Application date
- Application type
- Dosage of active substance
- Tillage dates

Several application schemes can be included in the file. Figure A 9 shows an example of the app-file including one application scheme. Further schemes can be implemented at the end of the file.

8.10.2 The substance parameters

In the cmp-file, the substance-specific parameters are defined. Multiple substances can be implemented. The header of the file lists default parameters that are valid for all substances. These parameters can be overwritten by including them in the second part of the file that contains substance-specific parameters. Figure A 10 shows the header of the cmp-file and the substance-specific parameters for the GeoPEARL dummy compound A.

8.10.3 The list of scenarios to be used for simulations

In the lis-file, a list or a range of unique combinations can be defined which then will be used for the simulation runs. The file is optional and is only used in a specific application mode. Figure A 11 shows an example of the lis-file. The first table represents a range of unique combinations, the second table beginning with “*”a list of unique combinations.

8.10.4 The parameters to control the simulation runs

The geo-file is the main control file of GeoPEARL_DE. Here, information on the model version is available. The input and output files, the simulation modes, the options for each mode and the output options can be specified. Here, the evaluation depth for output results can be determined. For standard GeoPEARL_DE runs, it is set to 1 m according to FOCUS (2000). A detailed description of the file structure is beyond the scope of this document. The interested user is referred to the GeoPEARL manual for further information (Tiktak et al., 2003, 2004a). Figure A 12 shows an example of the geo-file.

8.10.5 The list of output parameters

In the ctr-file, options for the SWAP model as well as options for data output can be specified.

9 Results and discussion

GeoPEARL_DE can be used for the spatial evaluation of the behaviour of plant protection products with respect to leaching to groundwater in Germany. The performance and the handling of the German schematisation were tested as well as the coherence of the water balances and the soil properties (here, in particular, the organic matter content).

9.1 The physical representation of GeoPEARL_DE

According to the requirements of the application GeoPEARL, a spatial schematisation including a set of environmental scenarios and their parameterisation was generated for Germany. 7744 different scenarios represented by unique combinations of soil and weather data were created. This results in a set of 7764 ASCII files with a need of disc space of about 9 GB. Most of the files (7744) represent the met-files for each scenario. An overview of the created files is given in Table 16 on page 60.

9.2 Handling of GeoPEARL_DE

The schematisation of GeoPEARL_DE was tested using the following versions of the executable files:

- swap209e.exe, version 2.09e2, created on 05-Jan-2006
- GeoPEARL.exe, kernel version 1.7.4, created on 20-Jan-2006
- Pearlmodel.exe, created on 20-Jan-2006

The first simulation runs were carried out to test the behaviour of the application when parameterised with the German spatial schematisation. Aspects such as function of the schematisation and the control files, goodness of the parameterisation and the time need for the simulations were investigated. Regarding the function of the files, it can be stated that the spatial parameterisation is ready to use. The dimension of the files (7764 with a disc space of about 9 GB) is not a critical issue regarding the processing of the simulations. Nevertheless, for model runs, a machine with a disc space of at least 10 GB is required taking into account the parameterisation and the temporary files.

The time need of one complete simulation is remarkable. A single run including all 7744 scenarios requires up to several weeks if started on a single machine. When testing the model using a new, fast machine (Intel Pentium 4 HT, 3.2 GHz, 1 GB RAM), the time need was estimated up to 30 days. The actual calculation time is influenced by the number of substances to be calculated, the speed of the machine and the additional work performed on the machine. Having tested the model, it can be stated that the calculation time is not equal for each scenario due to the different parameterisation and the differences between single scenarios are very high (from 44 seconds up to 6 hours). The differences are caused by SWAP. In some cases, SWAP needs to make calculations for very small time-steps to find a solution for the hydrology. Computing a large number of small time-steps leads to a longer computation time. However, the calculation time of PEARL is not critical. Because of the time needed, it is recommended to start simulation runs on more than one machine. For that purpose, the model application and the spatial schematisation can be installed on several computers. In the lis-files of each machine, a different range of UC ID’s can be defined and the runs can be started separately.

After termination of the simulations, the output files can be easily joined and analysis can be carried out. An overview of the output files is given in Appendix C.

9.3 The spatial schematisation

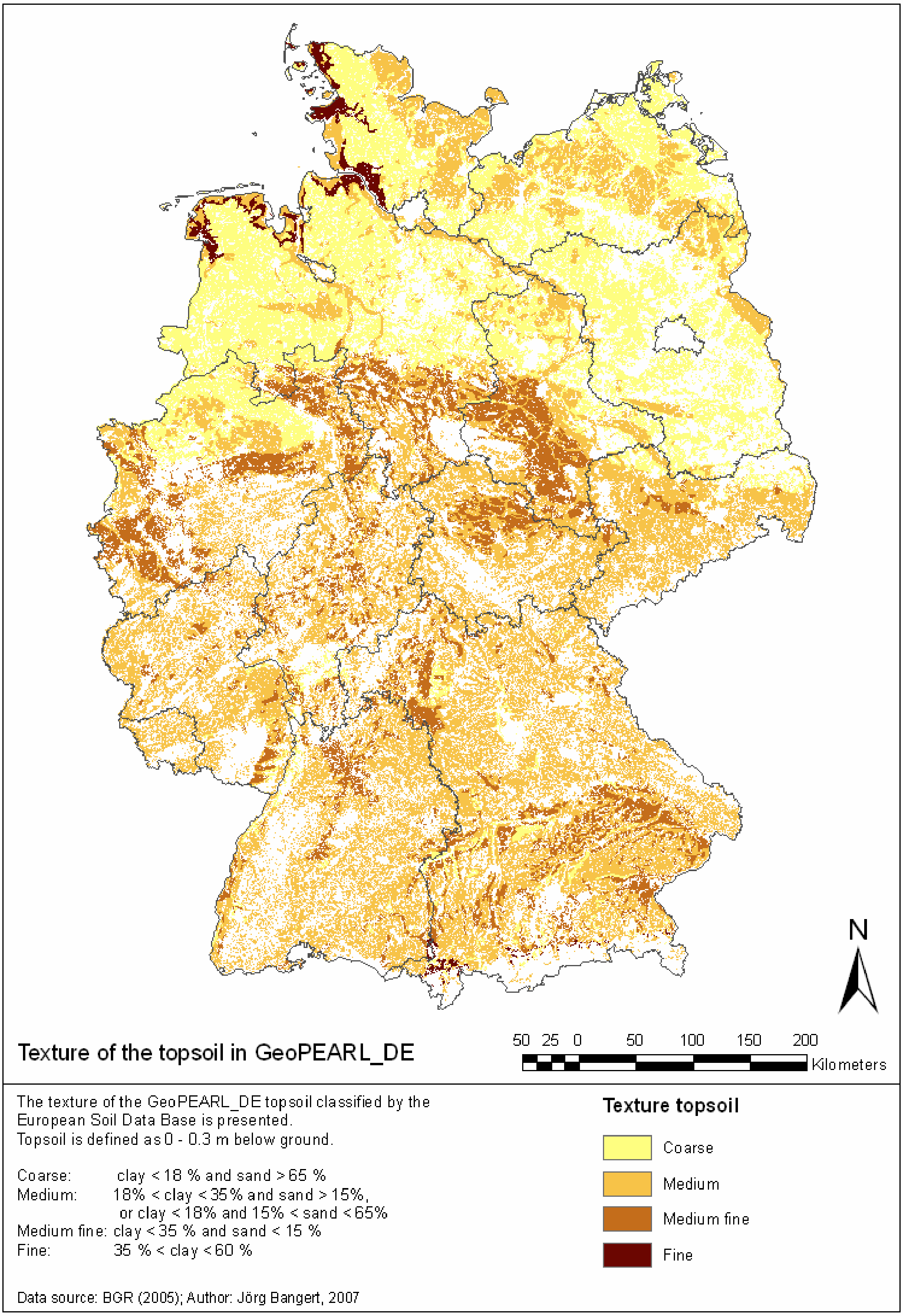
In the following section, the spatial schematisation of GeoPEARL_DE is presented and analysed. Some results are compared with other data sets to show if they present a realistic approach to the German situation. In this context, the evaluation of the hydrology is a very important issue of the following analysis because of its important influence on the leaching of a chemical into groundwater. For discussion of the hydrology, the German hydrological atlas (HAD, Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003) was used as a source of data to which the GeoPEARL_DE results are related. The GeoPEARL_DE results are not compared with measured field data because a comprehensive data set of the German hydrology situation which was gathered by field measurements was not available for this study. Thus, the HAD data sets, which were derived using modelling and interpolation approaches, are used for the analysis. These data also show limitations and restrictions regarding their implemented information which are caused by their theoretical background. Nevertheless, due to the sophisticated modelling assumptions and the implementation of the results of several point data from the field into the modelling approach, these data sets can be considered as an appropriate approach to the reality. However, they should not be regarded as an exact representation of the reality. Comparison was only possible on a “visual” basis because, for this study, the data of the HAD were not available to perform spatial analysis in a GIS.

The description of the soils in GeoPEARL_DE is based on the data of the German soil map BÜK 1000 (BGR, 2005, 2006). A comparison to other data sets was not necessary because the soil data such as texture and organic matter content are not simulated by the model but reflect the information of the soil profiles implemented in the BÜK database.

9.3.1 Soil texture

Figure 32 shows the texture classes of the topsoil as implemented in the GeoPEARL_DE schematisation. In the map, the sandy soils of northern Germany, which are vulnerable for leaching because of the coarse soil texture, are visible. The finest soils are located at the German North sea coast and at some small locations near the Alps. Furthermore, the soils with a higher fraction of loess are visible as soils with a medium fine texture.

The soil information of GeoPEARL_DE is based on a relative small number of soil profiles compared to the area of Germany and the actual variability of German soils. Furthermore, only classified data were available in the BÜK database. Thus, the map of the GeoPEARL_DE soil texture shows only a coarse pattern of the soil properties in Germany. It is recommended to increase the number of available soil profiles for the German schematisation to reflect the actual variability of the German soils in a better way.



The texture of the GeoPEARL_DE topsoil classified by the European Soil Data Base is presented.
Topsoil is defined as 0 - 0.3 m below ground.

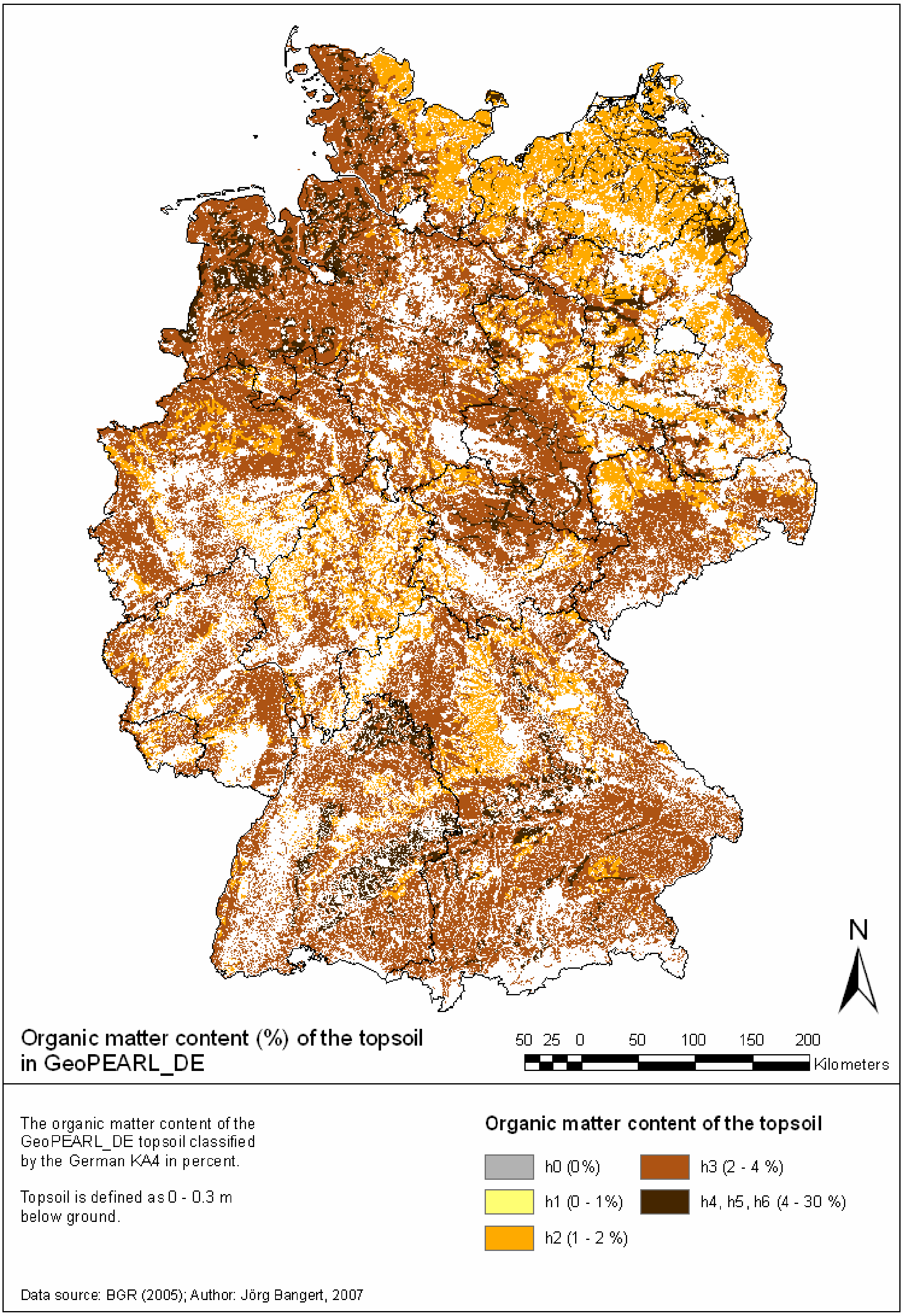
Coarse: clay < 18 % and sand > 65 %
Medium: 18% < clay < 35% and sand > 15%,
or clay < 18% and 15% < sand < 65%
Medium fine: clay < 35 % and sand < 15 %
Fine: 35 % < clay < 60 %

Data source: BGR (2005); Author: Jörg Bangert, 2007

Figure 32: Texture class of the topsoil in GeoPEARL_DE

9.3.2 Organic matter content

Figure 33 and Figure 34 show the organic matter content of the topsoil (0 - 30 cm) and the subsoil (30 - 100 cm) as implemented in GeoPEARL_DE.



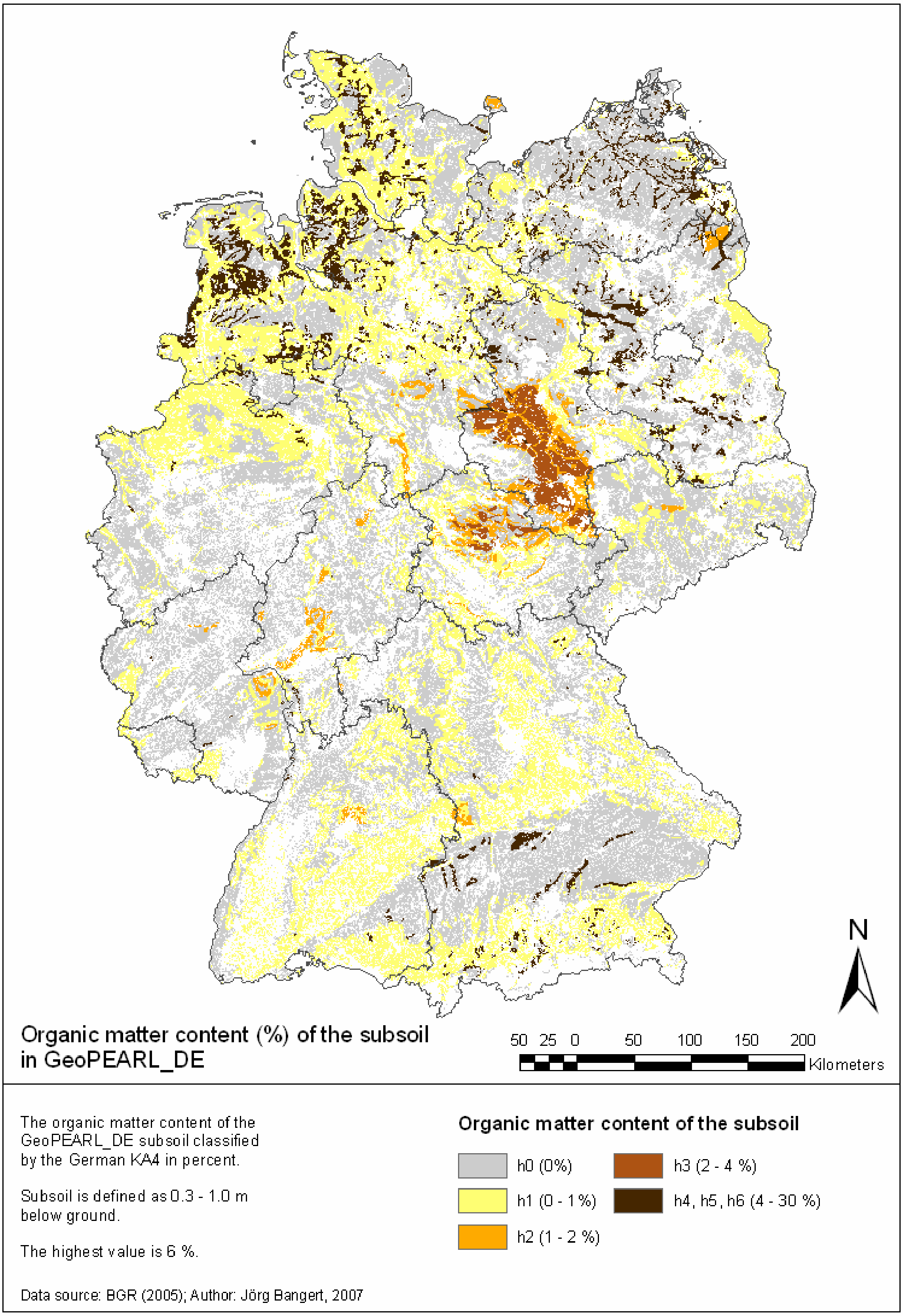
Organic matter content (%) of the topsoil in GeoPEARL_DE

The organic matter content of the GeoPEARL_DE topsoil classified by the German KA4 in percent.

Topsoil is defined as 0 - 0.3 m below ground.

Data source: BGR (2005); Author: Jörg Bangert, 2007

Figure 33: Organic matter content of the topsoil in GeoPEARL_DE



The organic matter content of the GeoPEARL_DE subsoil classified by the German KA4 in percent.

Subsoil is defined as 0.3 - 1.0 m below ground.

The highest value is 6 %.

Data source: BGR (2005); Author: Jörg Bangert, 2007

Figure 34: Organic matter content of the subsoil in GeoPEARL_DE

The organic matter (OM) content in the soil is an important parameter for the estimation of the leaching of a chemical to groundwater. As substances can adsorb to the soil particles and especially to the organic matter, a high OM content reduces leaching. Therefore, the evaluation of the humus parameter in the spatial schematisation is an important task of the analysis. The map of OM content in the subsoil (0.3 - 1 m) shows a value of zero in large regions of Germany. These values derive from the parameterisation given by the German soil profiles database (BGR, 2005). Here, for many soil profiles, the data class “h0” is defined. The substitution of the class value “h0” with a organic matter content of 0 % is seen as a critical issue because minimal fractions of humus, which can exist in the soil although the field observation did not find them, were not considered. This assumption was checked by the investigation of several actual soil profiles which were described in field and afterwards analysed in the laboratory (Altermann (1995), Sticher (1997), Beyme et al. (1999), Frielinghaus et al. (2003), Felix-Henningsen et al. (2005)). The analysis shows that the organic matter content of subsoils is actually not 0 % although the field observation resulted in the class “h0”. Thus, the current parameterisation of GeoPEARL_DE is not considered to reflect the humus content in a realistic way: It is assumed that it is underestimated, which influences critically the leaching simulation in the model, and the leaching amounts into groundwater are overestimated. A comprehensive evaluation and comparison with actual soil profiles goes beyond the scope of this study and should be subject of further improvements of the GeoPEARL_DE schematisation.

9.3.3 Potential evapotranspiration

Figure 35 shows the mean annual potential evapotranspiration as given in the MARS data. They are equivalent to values implemented in GeoPEARL_DE. In Figure 36, the same theme as given in the German hydrological atlas (HAD, Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003) is presented.

The maps show a very different picture of the potential evapotranspiration. One aspect is the different resolution of the data sets. The MARS tiles show evapotranspiration values for 50 km x 50 km tiles whereas the HAD data are based on a 1 km x 1 km raster. Furthermore, the values included in the MARS tiles are higher as the values of the HAD in general. This is caused by the different derivation methods. The values included in the MARS approach were derived by a method developed by Penman (van der Goot et al., 2003) whereas the HAD data originates from an approach of Wendling (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003). In the description of the HAD, it is indicated that the Penman approach leads to higher evapotranspiration amounts as the approach of Wendling as tested in previous studies. It can be concluded that the MARS data which were used in the GeoPEARL_DE parameterisation show a higher potential evapotranspiration as expected regarding the information in the HAD. The pattern of the values is quite difficult to compare because of the very different resolution. The regions of high values in the south-west and the east of Germany are echoed in some MARS tiles covering the respective region.

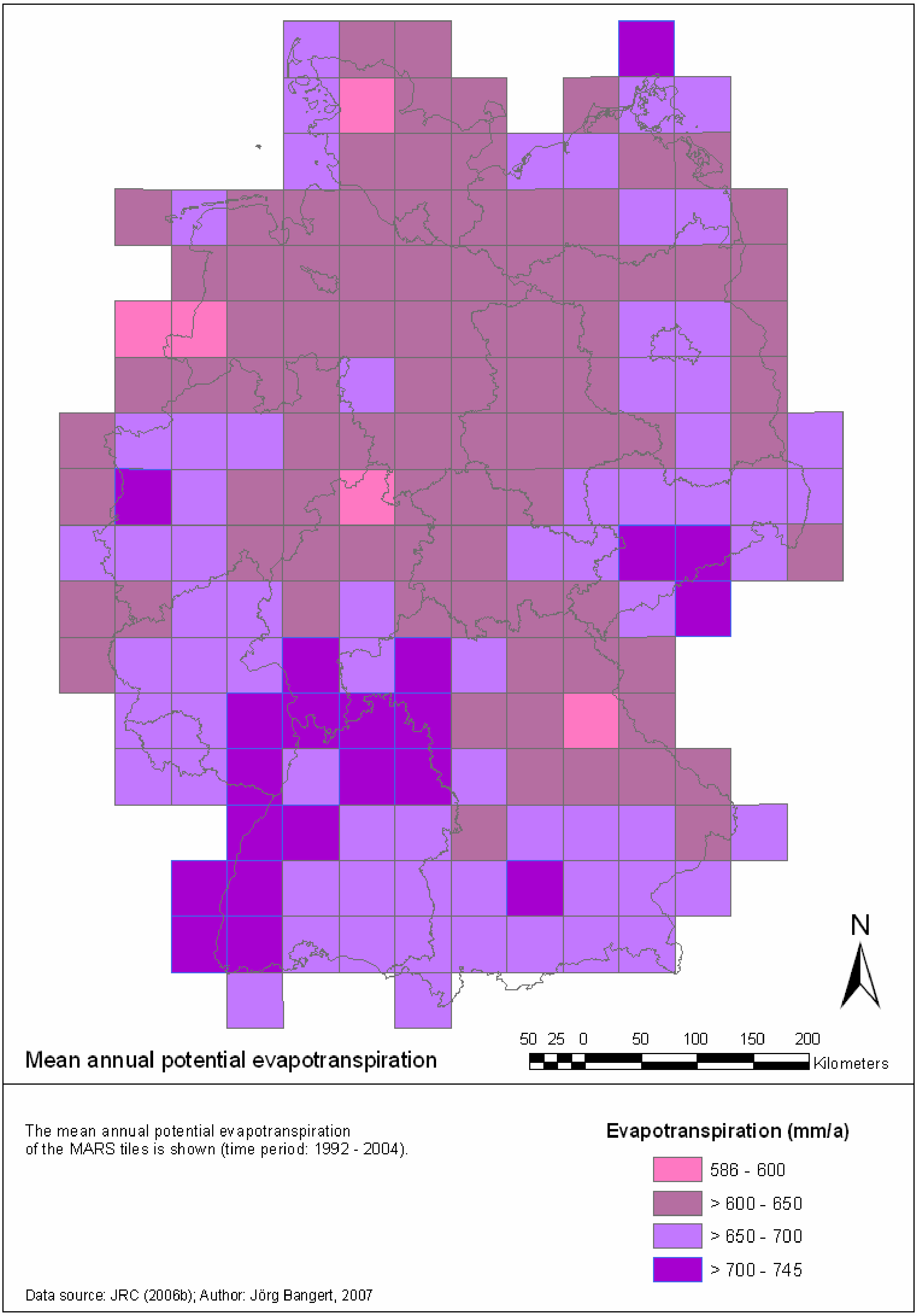
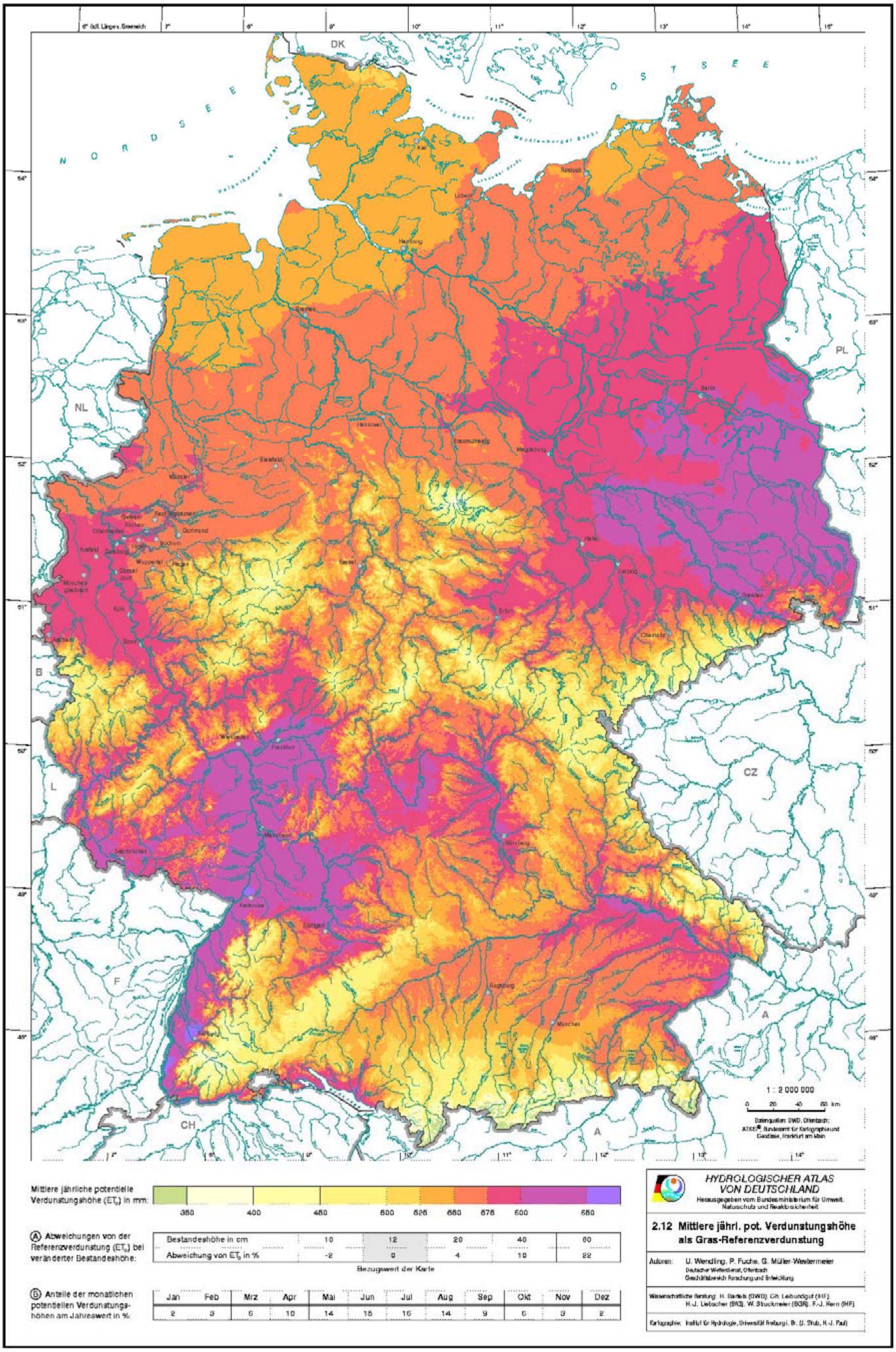


Figure 35: **Mean annual potential evapotranspiration according to MARS**



Datenquellen: DWD, Offenbach; ATKIS®, Bundesamt für Kartographie und Geodäsie, Frankfurt am Main

Ⓐ Abweichungen von der Referenzverdunstung (ET_0) bei veränderter Bestandeshöhe:

Bestandeshöhe in cm	10	12	20	40	60
Abweichung von ET_0 in %	-2	0	4	10	22

Bezugswert der Karte

Ⓑ Anteile der monatlichen potentiellen Verdunstungshöhen am Jahreswert in %

Jan	Feb	Mrz	Apr	Mai	Jun	Jul	Aug	Sep	Okt	Nov	Dez
2	3	5	10	14	15	15	14	9	5	3	2

2.12 Mittlere jährl. pot. Verdunstungshöhe als Gras-Referenzverdunstung

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Kartographie: Institut für Hydrologie, Universität Freiburg i. Br. (J. Stub, H.-J. Paul)

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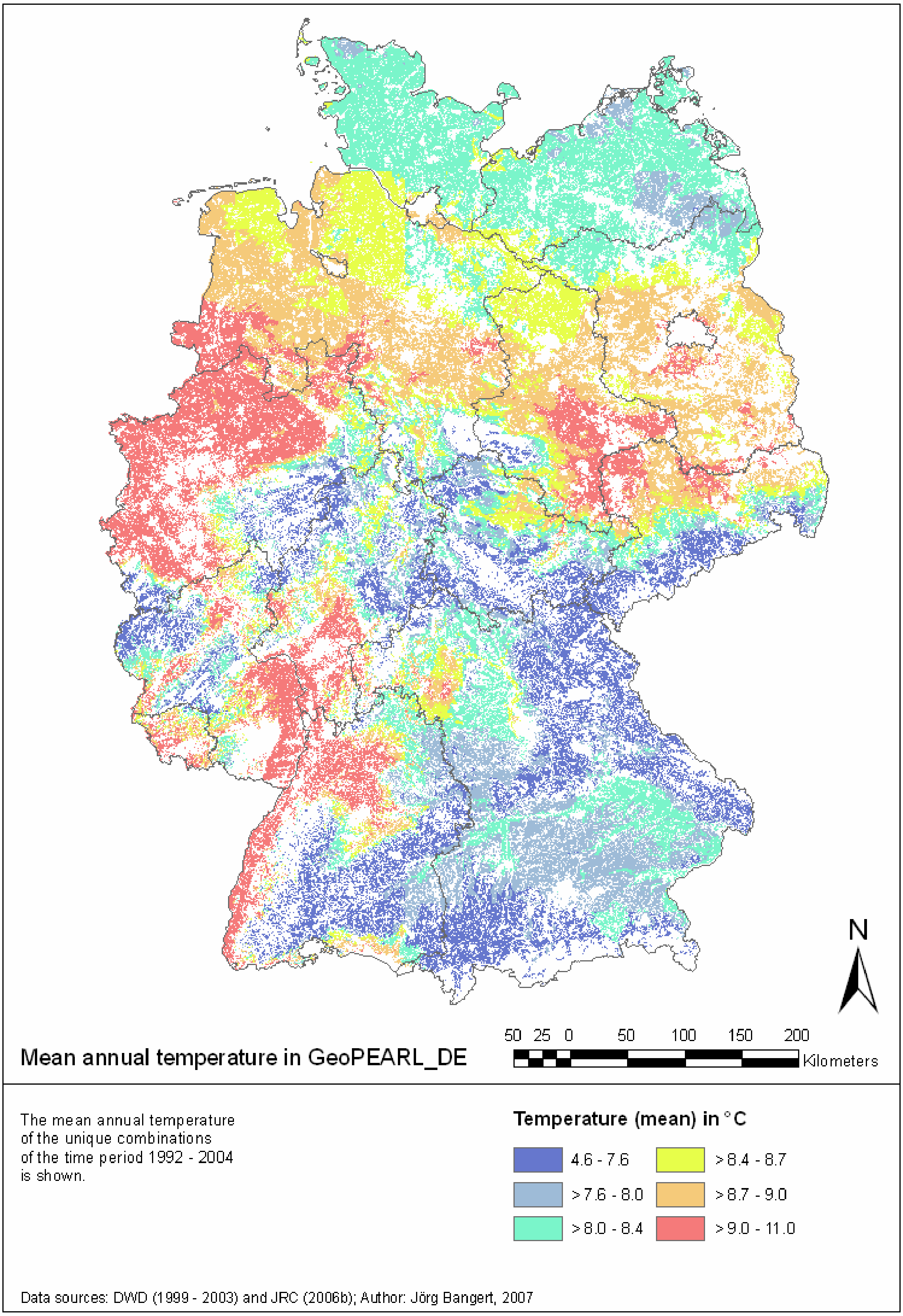
Figure 36: **Mean annual potential evapotranspiration according to HAD (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003)**

As the German weather service has not provided long-term values of the potential evapotranspiration, the MARS data could not be scaled to the high resolution of 1 km x 1 km. In a further improvement of the German schematisation, it should be considered to use the data of the HAD presented here to obtain a data set that is more appropriate to the scale of GeoPEARL_DE.

9.3.4 Temperature and precipitation

Figure 37 shows the mean annual temperature of the 13 years period implemented in GeoPEARL_DE. The presented pattern corresponds to the pattern presented in other official data sets, e.g. the map of long-term values provided by the German weather service (DWD, 1999 – 2003, see Figure A 5). In Figure 38, the mean annual sum of precipitation derived from the 13 years period of the German schematisation is presented. The comparison to the data sets provided by the German weather service (DWD, 1999 – 2003, see Figure A 4) and the HAD (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003) shows that the data used in GeoPEARL_DE give a good approach to the reality. However, in some regions, the borders of the MARS tiles become apparent (south Germany) which is caused by very different amounts of precipitation between the adjacent MARS tiles. For the purpose of the application, this phenomenon is not critical.

The good concordance of the temperature and the precipitation is due to the scaling procedure of the MARS data to the resolution of the DWD data as depicted in chapter 8.4 and Appendix B. Therefore, it can be concluded that the basic climate parameters temperature and precipitation represent a good approach to the German climate situation.



Mean annual temperature in GeoPEARL_DE

The mean annual temperature of the unique combinations of the time period 1992 - 2004 is shown.

Data sources: DWD (1999 - 2003) and JRC (2006b); Author: Jörg Bangert, 2007

Figure 37: Mean annual temperature according to GeoPEARL_DE

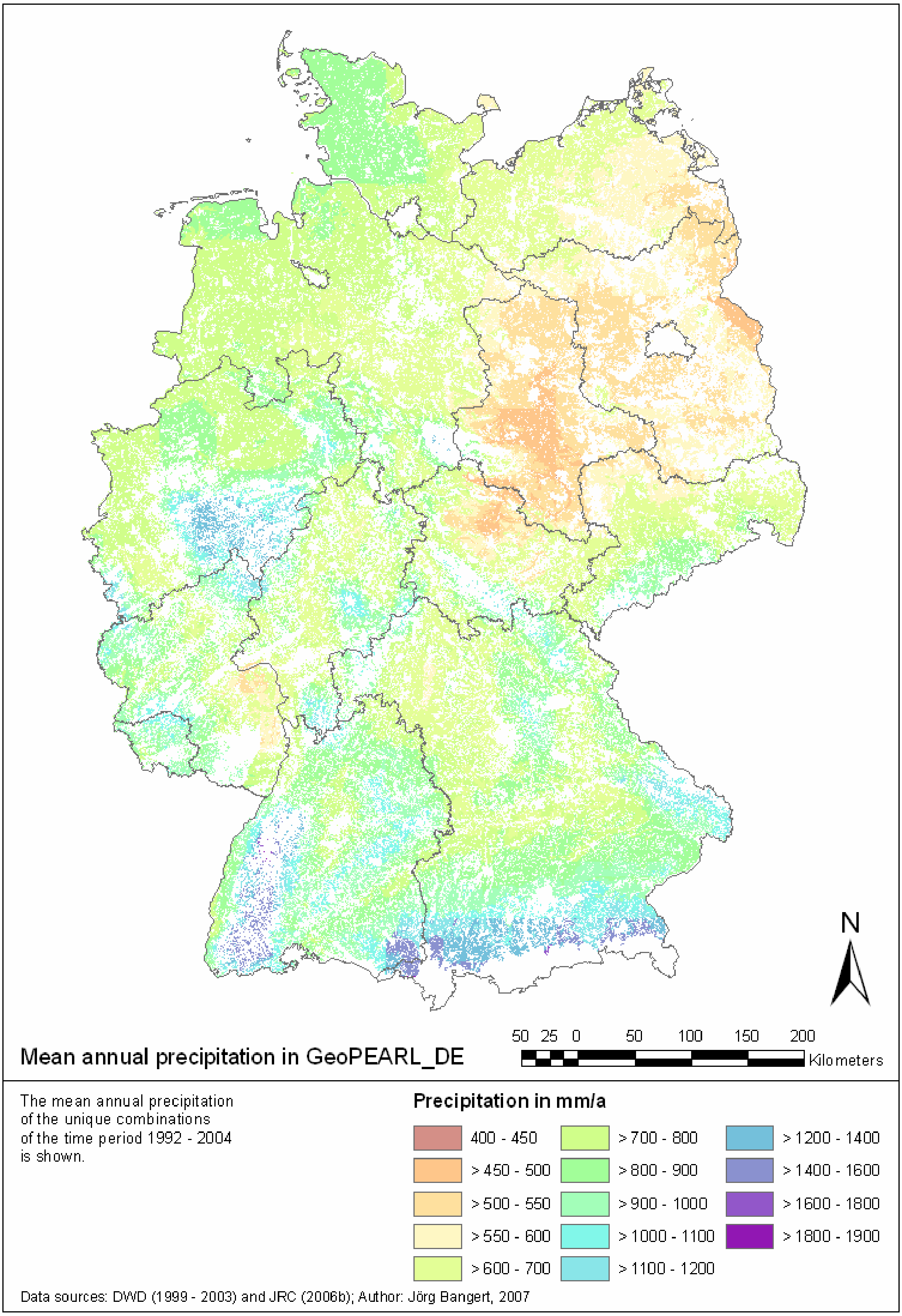


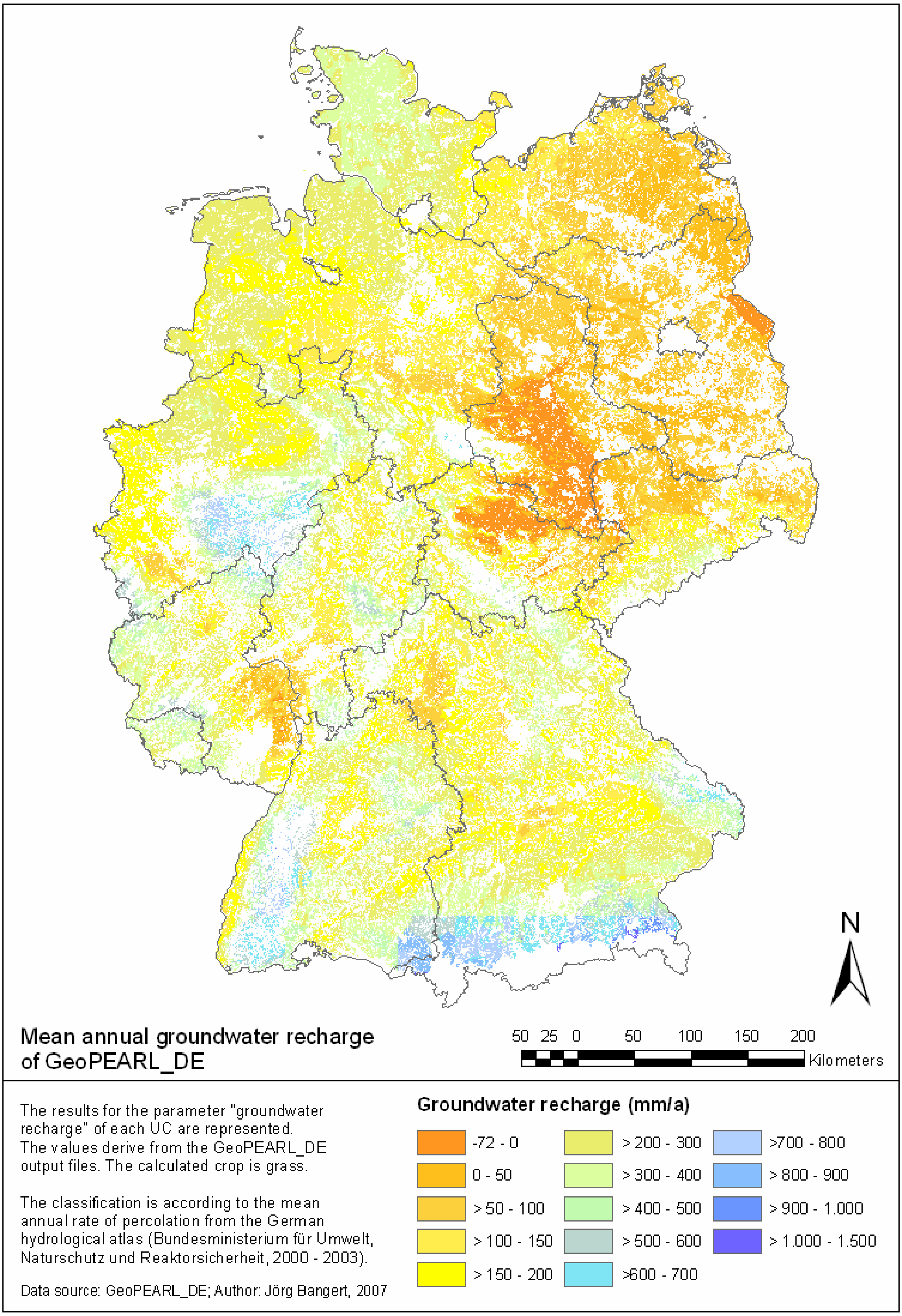
Figure 38: **Mean annual sum of precipitation according to GeoPEARL_DE**

9.3.5 Hydrology

The evaluation of the spatial schematisation should particularly consider the hydrological results as the soil-water system is not completely described in PEARL because of the lack of data on the drainage systems. The attention will turn to the output value of the groundwater recharge because it represents the input into the "target object" regarding the purpose of the application. In GeoPEARL, the groundwater recharge is calculated by integrating the simple difference of the incoming water (precipitation and irrigation) and the outgoing water (evaporation, transpiration, discharge to drainages and runoff) over the phreatic groundwater table (Tiktak et al., 2003). Actual evaporation and transpiration are calculated in the PEARL model by multiplying the potential evapotranspiration with specific soil and crop factors. The discharge of water to drainages is set to zero in all cases because of the lack of drainage data. Runoff is defined as the amount of water that ponds more than 1 mm on the soil surface. PEARL assumes the time period of the precipitation events of 24 hours a day, i.e. the daily amount of precipitation is distributed over 24 hours. Thereby, the intensity of rainfall events is underestimated as well as the amount of runoff because there is more time available for the infiltration then in reality when rainfall events last only several hours. Furthermore, the slope is not considered for the estimation of the runoff which leads to misestimations in general. If the water discharge to drainages and the amount of runoff water is underestimated, the amount of water reaching the groundwater – the groundwater recharge – is overestimated. As the groundwater recharge and the amount of substance that reaches the groundwater are coupled, an overestimation of the groundwater recharge can lead to a false simulation of the substance concentration in the groundwater. Thus an evaluation of the groundwater recharge is required.

The hydrological atlas of Germany (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003) offers spatial information on the percolation and on the groundwater recharge for Germany. In the HAD, the percolation is defined as the amount of soil water that leaves the soil downwards including the amount reaching the groundwater as well as the interflow. It is influenced by the parameters "precipitation", "irrigation", "capillary rise of water from the groundwater" (which are considered as input parameters) and the parameters "evapotranspiration" and "runoff" (which reduces the percolation amounts). The percolation information presented by the HAD is based on model assumptions and different data on soil and climate. The groundwater recharge represents the amount of soil water that reaches the groundwater which is in general defined as the percolation minus the interflow. The groundwater recharge shown in the HAD is also derived with the help of modelling approaches but using other methods as implemented in the derivation of the percolation.

In Figure 40, the mean annual rate of percolation from the soil and in Figure 42, the groundwater recharge is given according to the HAD. Figure 39 and Figure 41 show the same data set, which is the result of a GeoPEARL_DE simulation run referred to as "groundwater recharge" and presented according to the classification of the percolation (in the first figure) and the groundwater recharge (in the second figure) in the HAD, respectively.



The results for the parameter "groundwater recharge" of each UC are represented. The values derive from the GeoPEARL_DE output files. The calculated crop is grass.

The classification is according to the mean annual rate of percolation from the German hydrological atlas (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003).

Data source: GeoPEARL_DE; Author: Jörg Bangert, 2007

Figure 39: Mean annual groundwater recharge: results of GeoPEARL_DE, classified according to the mean annual rate of percolation from the soil of the HAD (see Figure 40)

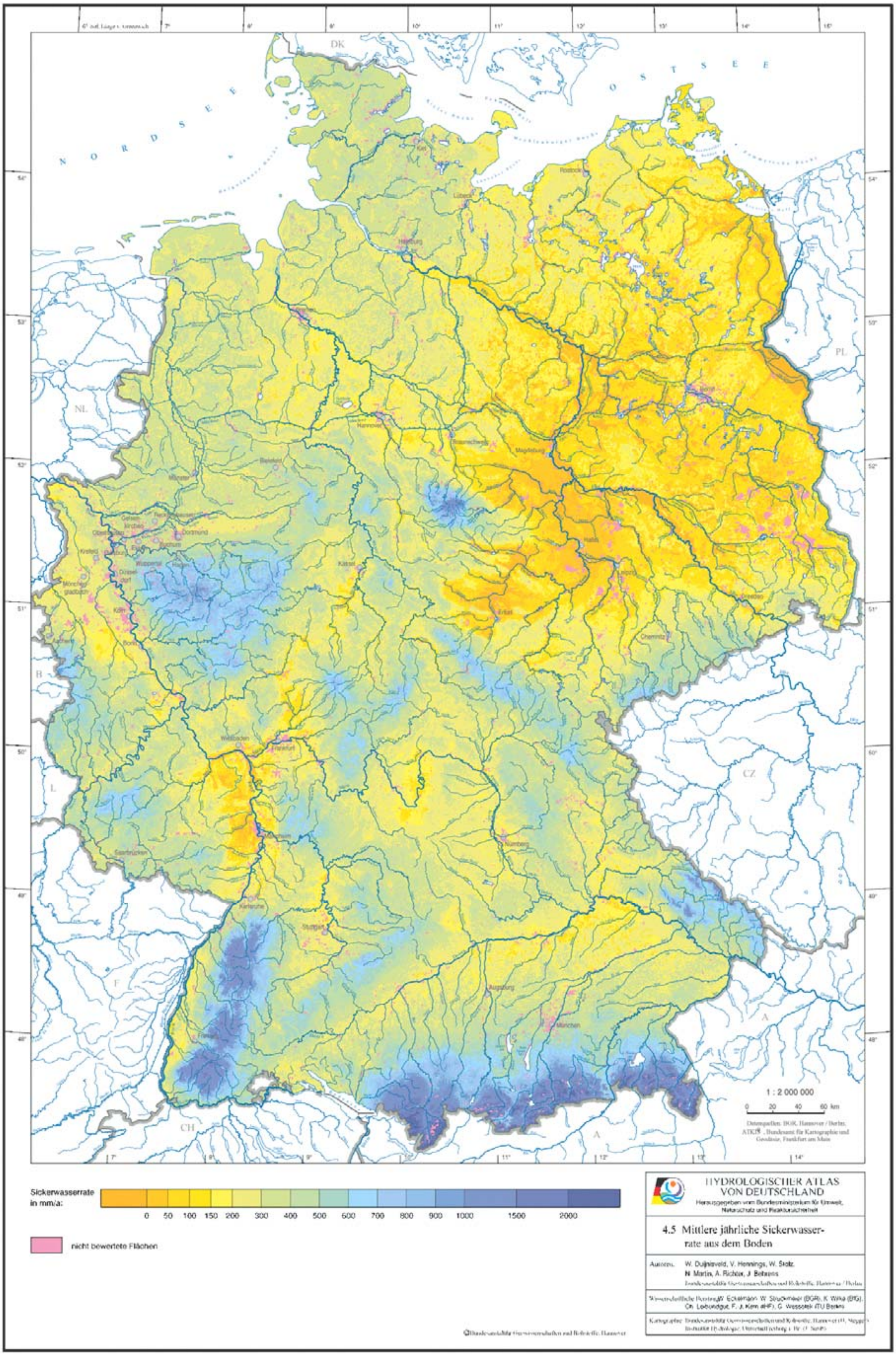


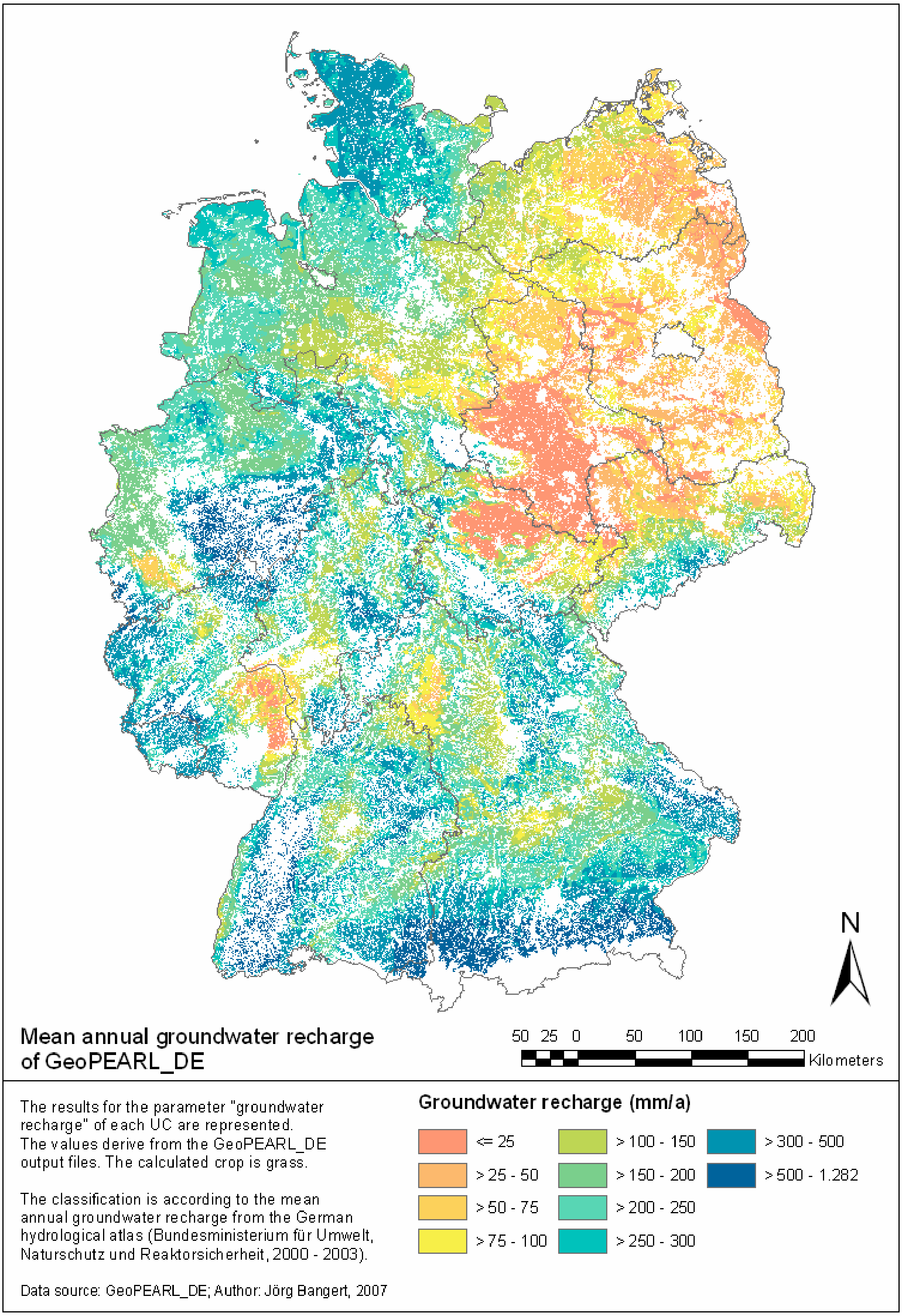
Figure 40: Mean annual rate of percolation from the soil according to HAD (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003)

Regarding the different definition of percolation and groundwater recharge as given in the HAD, the item “groundwater recharge” in GeoPEARL_DE is referred to as percolation: The percolation represents the sum of lateral discharges and the groundwater recharge (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003). As in GeoPEARL_DE no lateral discharges are implemented, the resulting values for groundwater recharge can be considered as percolation.

Figure 39 and Figure 40 show a similar pattern and similar amounts of the percolation rate in the HAD and the output data of GeoPEARL_DE classified according to the percolation map of the HAD. The mean values for whole Germany are 316 mm a^{-1} for the HAD data and 199 mm a^{-1} for the GeoPEARL_DE results. The differing mean values can be explained by the missing raster cells with high percolation rates in the spatial schematisation of GeoPEARL_DE, e.g. in the German Alps. They were excluded from calculations during the derivation of the area of interest because they are not covered by agricultural land use.

In Figure 41 and Figure 42, the groundwater recharge as given by GeoPEARL_DE and the HAD is represented. The map of the GeoPEARL_DE results shows a similar pattern but a higher amount of recharge values than the map of the HAD, especially in the regions at the coast, in the low mountain ranges and in the Alpine foothills. This leads to the assumption that in GeoPEARL_DE, the amounts of soil water reaching the groundwater are overestimated. Furthermore, with respect to the high potential evapotranspiration, it can be expected that the amounts will increase if the potential evapotranspiration will be improved in future applications. Lower values will be simulated if the lateral discharges such as drainages, runoff or interflow will be described in the model in a more realistic way. The adaptation of the model concerning this subject is going beyond the scope of this study and has to be conducted by the developer team of the software.

Once more, it is advised that the data of GeoPEARL_DE and the HAD cannot be exactly compared with each other because of the different methods of data derivation. Furthermore, only a visual comparison is possible because the HAD data were not available for a spatial analysis in a GIS. Nevertheless, the tendency of both data sets is visible and the main differences can be outlined.



The results for the parameter "groundwater recharge" of each UC are represented. The values derive from the GeoPEARL_DE output files. The calculated crop is grass.

The classification is according to the mean annual groundwater recharge from the German hydrological atlas (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003).

Data source: GeoPEARL_DE; Author: Jörg Bangert, 2007

Figure 41: Mean annual groundwater recharge: results of GeoPEARL_DE, classified according to the mean annual groundwater recharge of the HAD (see Figure 42)

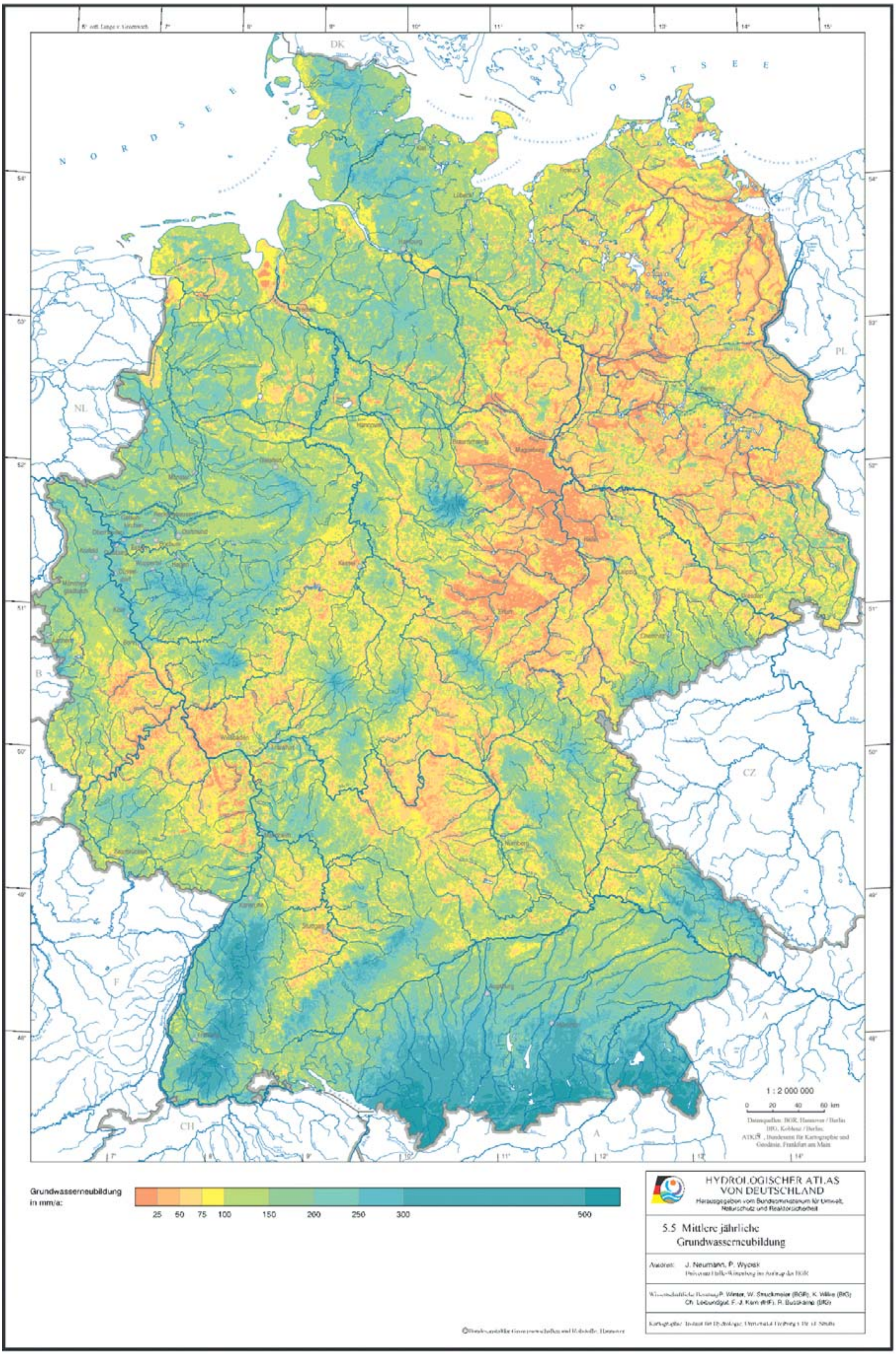


Figure 42: Mean annual groundwater recharge according to HAD (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, 2000 - 2003)

9.3.6 Conclusion of the spatial schematisation

Regarding the soil parameters implemented in GeoPEARL_DE, further adaptation is recommended for the organic matter content of the subsoil. It is considered to be too low for large regions of Germany. Investigations should be carried out to obtain more realistic values for the humus content of the subsoil. Furthermore, the number of soil profiles implemented in the spatial schematisation should be increased to implement a wider range of soil properties.

Summarising the climate and the hydrology as given in the GeoPEARL_DE scenarios, it can be asserted that the input parameters temperature and precipitation show realistic values. The potential evapotranspiration should be improved because of the very coarse resolution and the high values compared to the HAD data. In spite of the realistic input data (and the higher potential evaporation) the groundwater recharge calculated by GeoPEARL_DE is clearly overestimated. Therefore, it is recommended to improve the simulation methods within the model to describe lateral discharges in a more realistic way.

9.4 Differences to the Dutch approach

In comparison to the Dutch approach of GeoPEARL, the structure of the application, i.e. the required set of files, and the structure of the files have not changed. But, in several cases the function of a file or an option has changed.

The dra-file

The dra-file should include information on the drainage systems. As no information about this topic is available for Germany, the file is not parameterised and has currently no function in GeoPEARL_DE.

Linkage between scenario and simulated crop

Regarding the allocation of crops to unique combinations for a simulation, several differences between the German and the Dutch approach exist: In the Dutch approach, the link between the unique combination and the crop parameters that are used for the simulations is fixed because of restrictions of the Dutch parameterisation, i.e. simulations for a scenario are always carried out with the same crop parameters ignoring the crop used for scenario selection. These limitations are not necessary in the German approach. This leads to the following differences between the Dutch and the German approach:

1. crp-file

In the Dutch approach, one single crp-file exists which includes the parameters for all crops. Each crop is referred to an ID that represents the link to the plo-file. In the German approach, for each crop a single crp-file is available which contains one parameter set. The crop which should be used for calculations is defined in the geo-file by selecting the respective crp-file.

2. Link between scenario and crop

The link between scenario and crop is defined in the plo-file. In the crop type item, the ID of the crop as given in the crp-file can be set and thus, the defined crop is used for calculations. In the German approach, the standard value “1” is implemented. The standard value refers to the crop parameter set with the ID “1” in the crp-file. In the geo-file the crp-file is defined that has to be used for the simulations.

The mis-file

The mis-file in the Dutch approach contains the scenarios for which the model SWAP has no solution so it is possible to exclude them from model calculations. This makes sense because in the Dutch approach, the simulations for a scenario were always carried out with the same crop. In the German approach, the link between scenario and crop is not fixed and for different simulated crops different parameters are used in combination with a UC which results in different SWAP-solutions. Therefore, the definition of a fixed list of non-working UC for SWAP in GeoPEARL_DE is not possible. The function of the mis-file was changed and it is used for the elimination of scenarios which have no parameterisation regarding the soil properties as is described in chapter 8.9.

9.5 Uncertainty issues and model limitations

The German spatial schematisation for GeoPEARL was generated with care considering data accuracy, selection of an appropriate spatial resolution and comprehensive databases. However, the results show that the model outputs have to be handled carefully because of the variable sources of uncertainty and limitations of the model and the data sources.

The description of the environmental processes in the underlying model is one important source for uncertainty. The behaviour and limitations of the PEARL model are described in detail in Leistra et al. (2001). Therefore, in the work here presented, only a general overview of model uncertainty is given: The precision of a model simulation depends on the accuracy of the simulated process in comparison to the actual processes in the environment. If important process such as sorption or transformation are not comprehended exactly or are even ignored, the simulation results will not be realistic. For example, within PEARL, the process of preferential water flow in the soil along the tubes of earthworms is not implemented. Also, the process of runoff from the soil surface and the erosion of substances are not described in an appropriate way.

In general, the usage of a model is restricted to a determined range of environmental conditions from which the model processes were derived. Extrapolation away from the model range is a very critical issue because the results are not validated and misinterpretations are very common.

Further limitations and sources of uncertainty with respect to spatial modelling are given by the data sets and the methods which were used for the derivation of the scenarios. Tiktak et al. (2004b) described possible model errors which can result from the generation of the scenarios. The depicted error sources are also valid for the development of GeoPEARL_DE. The German schematisation describes the environment with 1 km x 1 km raster cells which are furthermore summarised to larger units – the unique combinations. Within one unique combination, the environmental parameters are considered to be equal which is a necessary simplification of the reality. Actually, soil and weather parameters vary in smaller distances than 1 km and they do not change abruptly at “hard” boundaries. Therefore, GeoPEARL ignores the variation of processes within one scenario. An approach to a more realistic description should lead to a very high spatial resolution. As no accordant data are yet available for such an approach, the current spatial schematisation represents the optimal description of the environment for a German-wide scale.

For the parameterisation of the soils in GeoPEARL_DE, the information provided in the soil database BÜK 1000 was used. Some parameters are given as classified data which were transformed into numerical values. Some parameters, such as the van Genuchten parameters, were not measured but derived from other soil parameters using pedotransfer functions. That means that the resulting soil profiles do not reflect the actual range of properties because many possible parameter values were ignored. Furthermore, the soil database provides only a limited number of profiles which obviously do not reflect the real range of the German soils.

The weather data used in the model were derived from a simple scaling procedure. This procedure only adapts the precipitation amount and the temperature for each unique combination. However, the weather calendar was not changed, i.e. for all scenarios, which are originated from the same MARS tile, the time of a precipitation event and the general trend of the temperature are equal. For a 50 km x 50 km raster this is not a realistic assumption. With respect to the time span between the application of a plant protection product and a precipitation event, this is a critical issue for the spatial pattern of modelling results. Having this fact in mind, it is coherent when the pattern of the MARS tiles is partially visible in the pattern of the resulting maps.

Based on the outlined limitations, the modelling results cannot be expected to give exact predictions for a certain point. This is an acceptable issue of the German spatial schematisation because GeoPEARL_DE should describe the range of environmental scenarios in agricultural used land in an adequate resolution with respect to a German-wide scale. The current parameterisation can be used for different analysis, e.g. to identify regions which are vulnerable for leaching of pesticides to groundwater with respect to the general climate and soil conditions. The model output can be analysed using statistical methods and conclusion for a German-wide range can be given.

With respect to the organic matter in the subsoil and the simulation of the groundwater recharge, the current parameterisation of GeoPEARL_DE represents a worst case as described in the previous section.

10 Future development and improvement

The application GeoPEARL_DE can be used for investigation of the leaching behaviour of pesticides in Germany using the spatial schematisation and the parameterisation as described in this document. Nevertheless, not all ideas and approaches could be realised with this version of GeoPEARL_DE. This section of the document will describe adaptations and approaches that can be implemented in future.

10.1 Parameter refinement

Considering the parameterisation of the GeoPEARL_DE scenarios, some future adaptations should be taken into account. In the existing version, no data on drainage or spatial differentiated groundwater levels are implemented because of the lack of appropriate data sets. If in future, the required spatial data sets become available, the information can be added to the respective files. Thereby, the simulation of the hydrology will be improved.

Currently, in the crp-files, only one crop parameter set is defined which is based on the crop parameters of the FOCUS groundwater scenario Hamburg. For further adaptations, it is possible to define multiple parameter sets for the same crop for different regions in the respective crp-file. The parameter sets are coded with different ID’s which then are assigned to the respective unique combination in the crop type item of the plo-file. For example, the scenarios located in North-Germany can be related to crop parameters which are appropriate for this region whereas for South-Germany, other parameters can be used for the simulations. The allocation can be conducted with respect to precipitation and temperature as presented in Table 3. The PEARL crop scenarios can be related to the scenarios showing the respective climate parameters. This option is not realised in the current version of GeoPEARL_DE but can be implemented in further extensions.

Regarding the soil data, improvements can be made by implementing new and advanced information on soil profiles. In the present version of the model, only soil profiles related to the land use “field crops” are parameterised. The van Genuchten parameters provided by the BGR (BGR, 2006) are only valid for this land use class. Thus, only calculations for application schedules using field crops can be carried out. If, in the future, calculations for substance applications in pastures should be required and the van Genuchten parameters for the land use class “pastures” are available for the BÜK data set, a further soil database can be created. Furthermore, investigations on the organic matter content in the subsoil are required because the current implementation results in too low values. This is a critical issue with respect to the leaching amounts as the mobility of agrochemicals is influenced by the humus content and leaching to the deeper soil can be retarded.

The statistical data used for the creation of the crop database (unc-file) were created in 2003. The official data sets are adapted in regular time intervals. Thus, it is possible to renew the data on cropping area in a few years.

10.2 Refinement of the spatial schematisation

If, in the future, new spatial data sets on climate, hydrology or soil become available which are more appropriate for use in the modelling context, a new spatial schematisation should be generated. The development of unique combinations based on this new information must consider the properties and constraints of these data and is only roughly comparable to the current approach. Setting up a new spatial schematisation will lead to a different result and is going beyond a simple parameter refinement. However, the implementation of improved data sets is an advancement of the scenarios used for spatial modelling. The next phrases give some examples of advanced data sets which might be available in the future: The development of a comprehensive German-wide soil map in the scale 1:200,000 (BÜK 200) will result in a new soil database which shows a higher level of detail and a higher spatial resolution as the BÜK 1000 data set which is used for the current version of GeoPEARL_DE. If comprehensive information on the drainage systems or the lower boundary conditions will become available for Germany, these data can be used for the development of new unique combinations and the additional information will improve the hydrology simulation of the model. The same effect will show the implementation of high resolution data of the potential evapotranspiration for Germany which are provided by the German atlas of hydrology.

Besides the refinement of the GeoPEARL_DE parameterisation, it is possible to develop a spatial schematisation for another country or a smaller region within Germany which would consider other data sets with a higher resolution.

10.3 Advanced program versions

Regarding the technical aspects of GeoPEARL, further adaptations can be expected. If new versions of the model executables are available, they can be used instead of the current files. Currently, the developer team of GeoPEARL is improving the calculation for runoff water. The new calculation method will lead to higher amounts of runoff water and to an improved description of the soil hydrology. However, it is recommended to determine that the new program versions do not require changes in the spatial schematisation or the control files, respectively.

11 Conclusion

For the evaluation of the leaching behaviour of plant protection products on a German national scale, a tool for spatial modelling of agrochemicals was developed – GeoPEARL_DE. The application is based on the modelling software GeoPEARL which was developed for decision support in the registration procedure of pesticides in the Netherlands. The software was adapted to the German situation by creating a new spatial schematisation, which is described in the here presented document, using German and European spatial data sets. The German schematisation is based on weather data provided by the German weather service and the MARS database. Soil information was taken from the German soil database BÜK 1000. Information on land use is available in the CORINE land cover data set and the area of cultivable land for a range of crops was derived from the database of the Federal Statistical Office of Germany. These data sets were combined to get a set of 7744 scenarios which represent unique combinations of environmental parameters. The scenarios were parameterised according to the requirements of the software using the data provided in the available databases.

The evaluation of the parameterisation focuses on the soil properties and the hydrology results. Despite the appropriate input data for temperature and precipitation and the high values for potential evapotranspiration, the model simulates a very high amount of water reaching the groundwater. This is caused by the misestimation of lateral discharges due to the lack of data on drainage systems and the underestimation of runoff at the soil surface by the original model implementation. Furthermore, the organic matter content in the subsoil is assumed to be too low with respect to realistic soil profiles. Therefore, it can be concluded that the current parameterisation of GeoPEARL_DE is not yet appropriate to predict environmental concentrations of pesticides. While the predicted environmental concentrations should be considered too conservative, the overall spatial pattern of leaching can be considered realistic and allows identifying, which regions are most vulnerable for leaching.

With respect to the limitations of the current parameterisation, further improvements are recommended. The organic matter content of the subsoil should be investigated and a parameterisation that demonstrates more realistic values should be developed. Regarding the hydrology, the internal description of runoff and lateral discharges in the model software should be changed to avoid unrealistic amounts of groundwater recharge. If data on drainage systems in Germany become available in future and if they are implemented into the parameterisation, the simulation of hydrology will be improved. Furthermore, the usage of the potential evaporation data provided by the HAD instead of the coarse MARS data should be taken into account.

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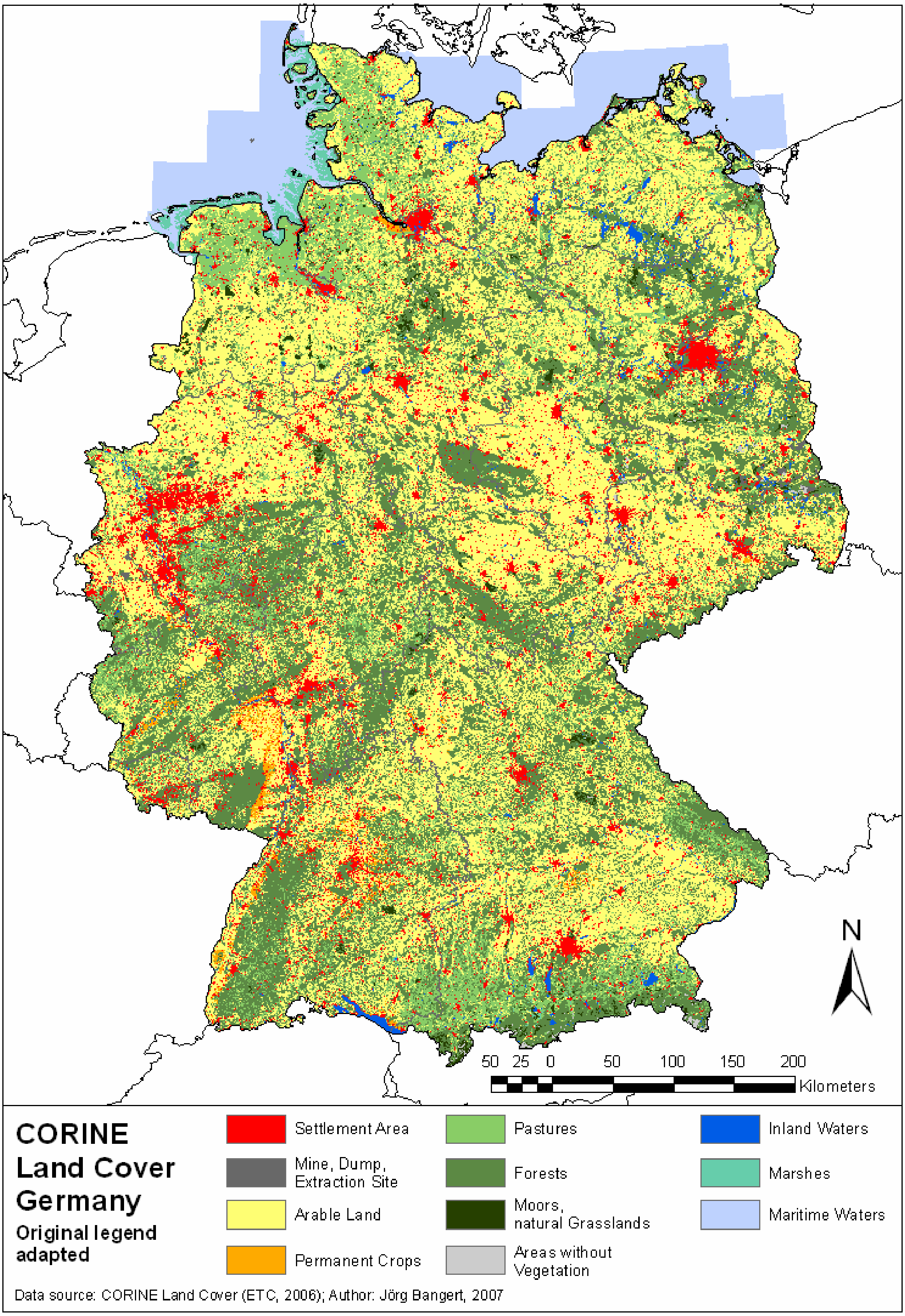
Appendix A: Figures and Tables



Data source: CORINE Land Cover (ETC, 2006); Author: Jörg Bangert, 2007

Figure A 1: **Map of the CORINE land cover**

Table A 1: Classification of the CLC data set

CODE2000	Description
1	**Artificial surfaces**
11	Urban fabric
111	Continuous urban fabric
112	Discontinuous urban fabric
12	Industrial, commercial and transport units
121	Industrial or commercial units
122	Road and rail networks and associated land
123	Port areas
124	Airports
13	Mine, dump and construction sites
131	Mineral extraction sites
132	Dump sites
133	Construction sites
14	Artificial, non-agricultural vegetated areas
141	Green urban areas
142	Sport and leisure facilities
2	**Agricultural areas**
21	Arable land
211	Non-irrigated arable land
212	Permanently irrigated land
213	Rice fields
22	Permanent crops
221	Vineyards
222	Fruit trees and berry plantations
223	Olive groves
23	Pastures
231	Pastures
24	Heterogeneous agricultural areas
241	Annual crops associated with permanent crops
242	Complex cultivation patterns
243	Land principally occupied by agriculture, with significant areas of natural vegetation
244	Agro-forestry areas
3	**Forest and semi natural areas**
31	Forests
311	Broad-leaved forest
312	Coniferous forest
313	Mixed forest
32	Scrub and/or herbaceous vegetation associations
321	Natural grasslands
322	Moors and heath land
323	Sclerophyllous vegetation
324	Transitional woodland-shrub
33	Open spaces with little or no vegetation
331	Beaches, dunes, sands
332	Bare rocks
333	Sparsely vegetated areas
334	Burnt areas
335	Glaciers and perpetual snow
4	**Wetlands**
41	Inland wetlands
411	Inland marshes
412	Peat bogs
42	Maritime wetlands
421	Salt marshes
422	Salines
423	Intertidal flats
5	**Water bodies**
51	Inland waters
511	Water courses
512	Water bodies
52	Maritime waters
521	Coastal lagoons
522	Estuaries
523	Sea and ocean

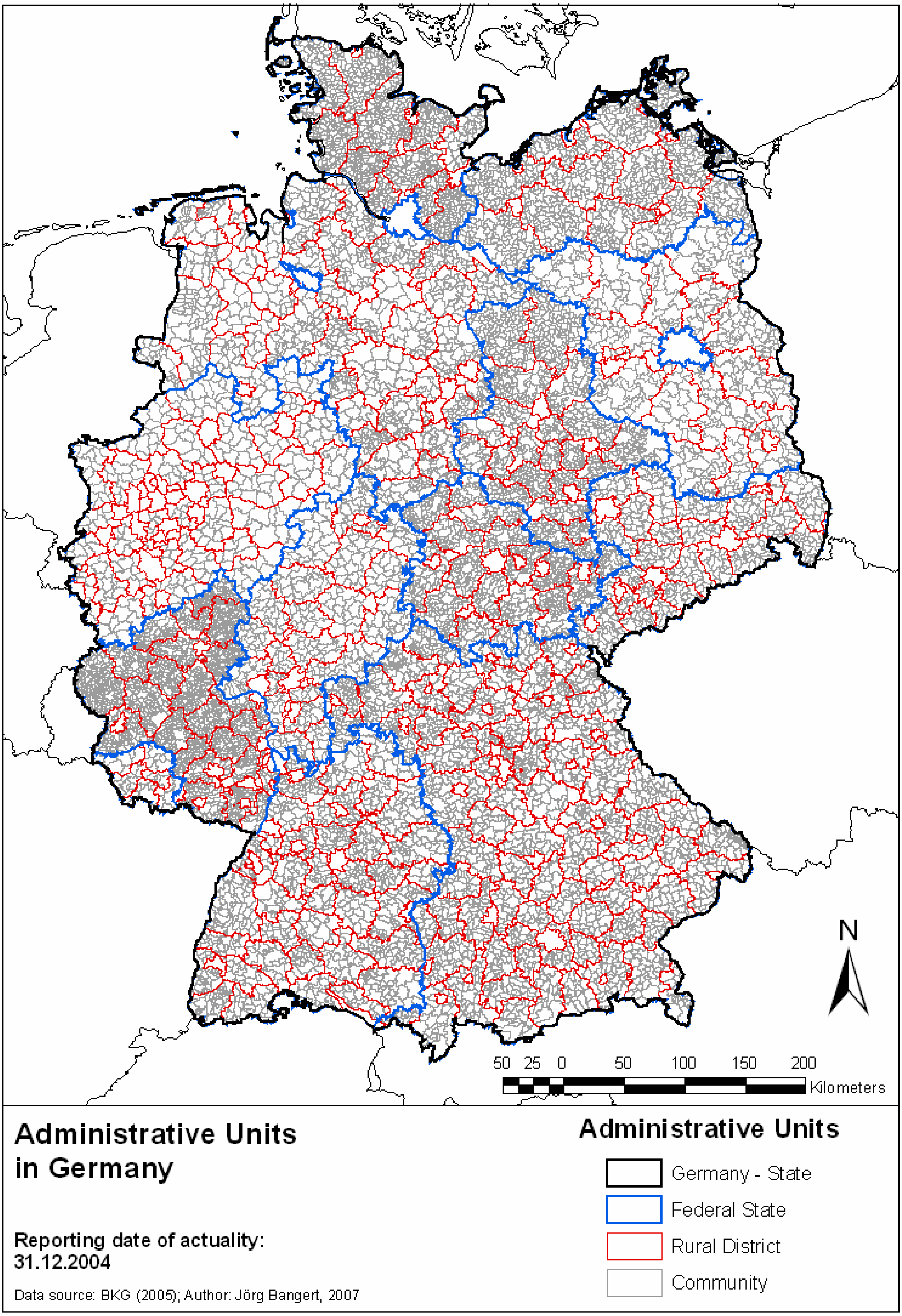
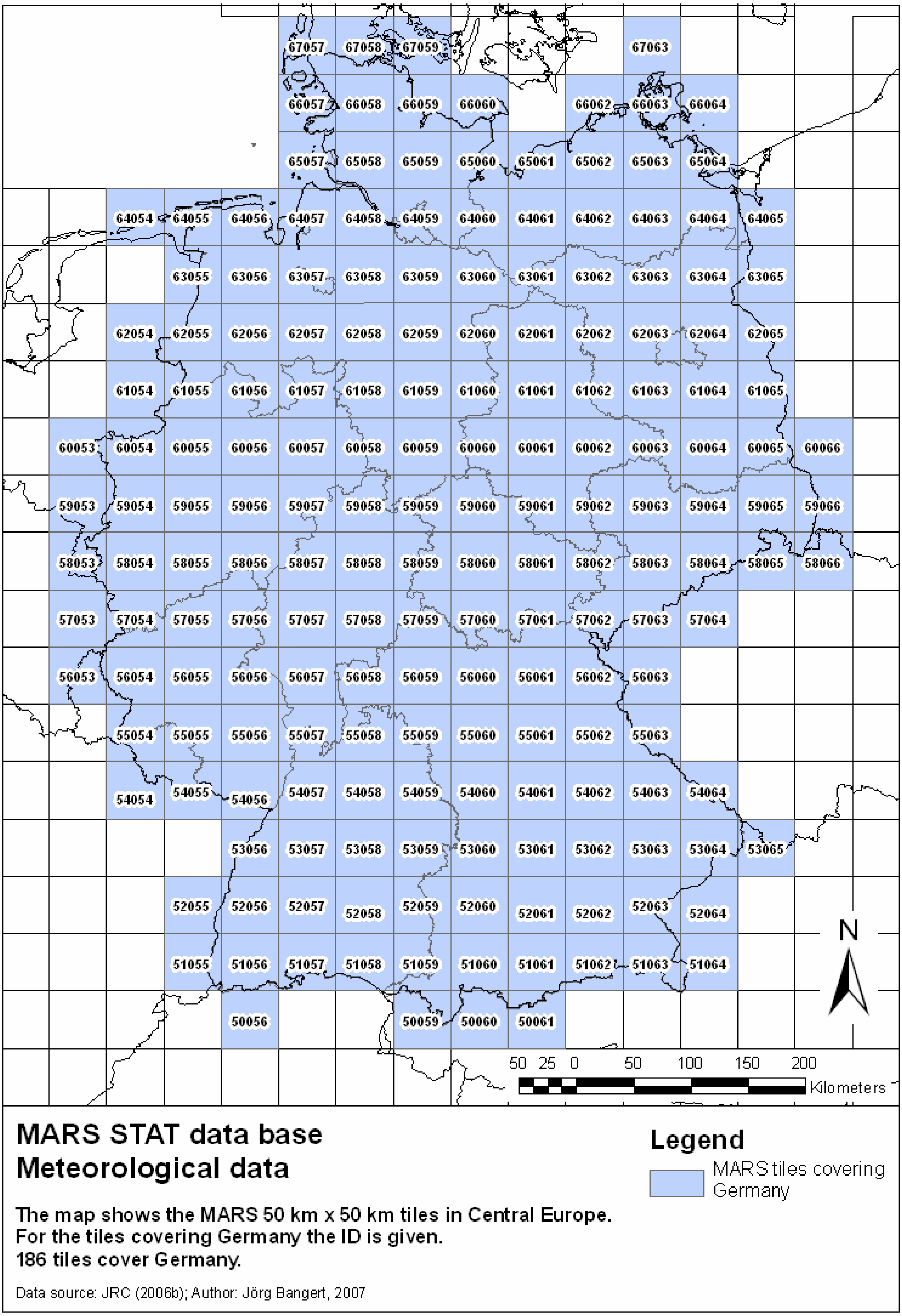


Figure A 2: **Map of the administrative units of Germany**



MARS STAT data base
Meteorological data

The map shows the MARS 50 km x 50 km tiles in Central Europe.
For the tiles covering Germany the ID is given.
186 tiles cover Germany.

Data source: JRC (2006b); Author: Jörg Bangert, 2007

Figure A 3: **Map of the MARS tiles covering Germany**

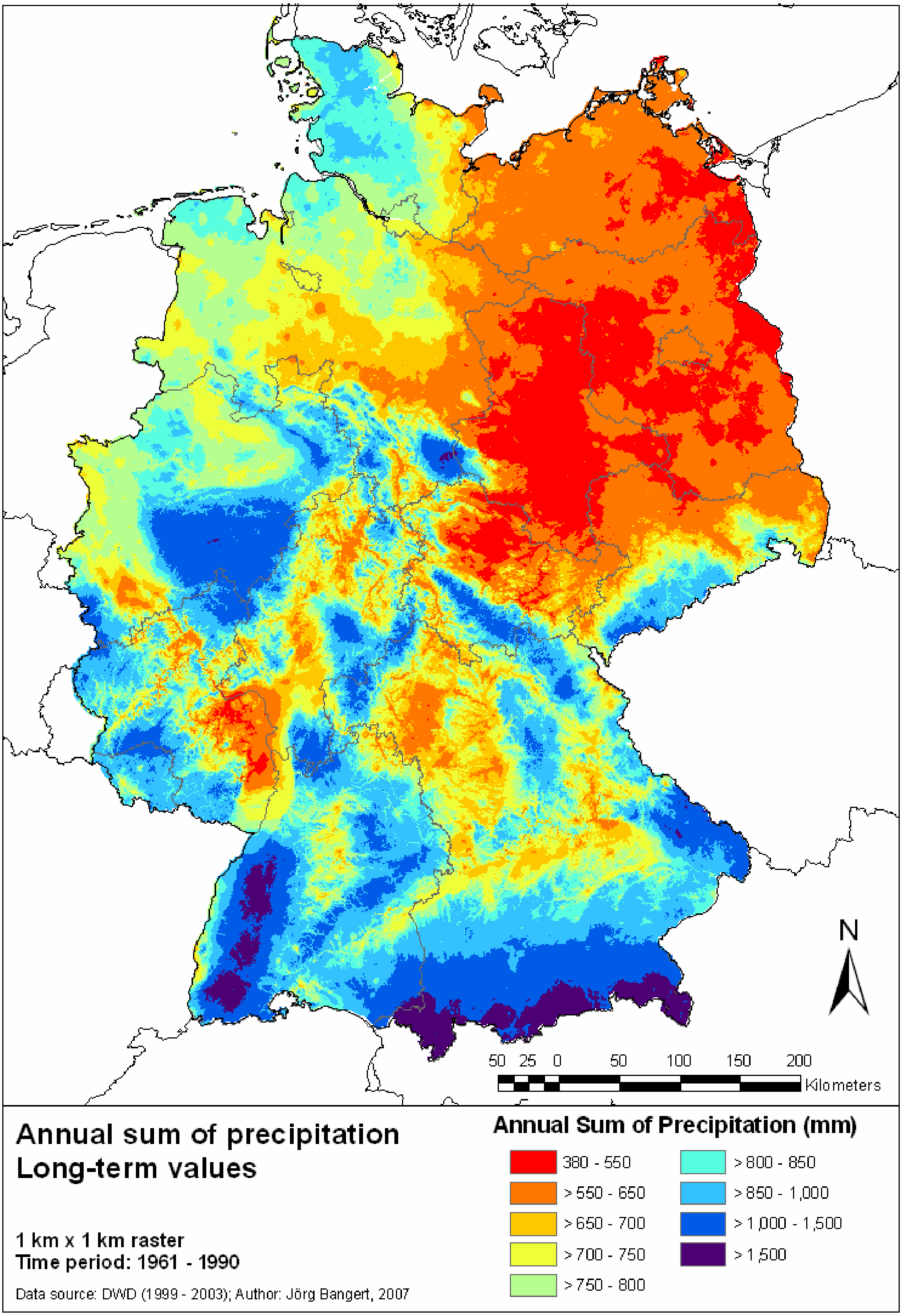


Figure A 4: Map of the DWD data set (annual sum of precipitation)

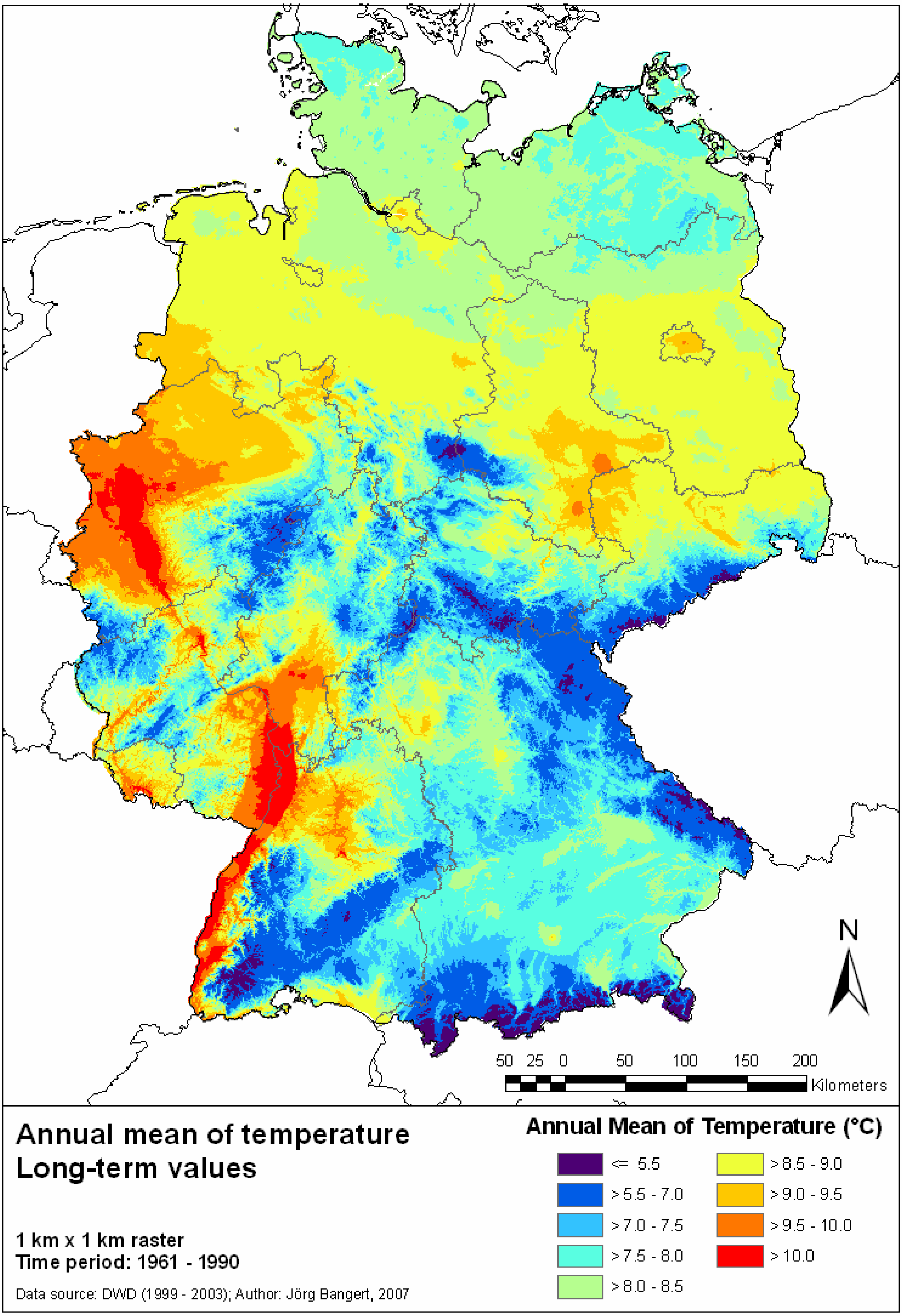


Figure A 5: Map of the DWD data set (annual mean of temperature)

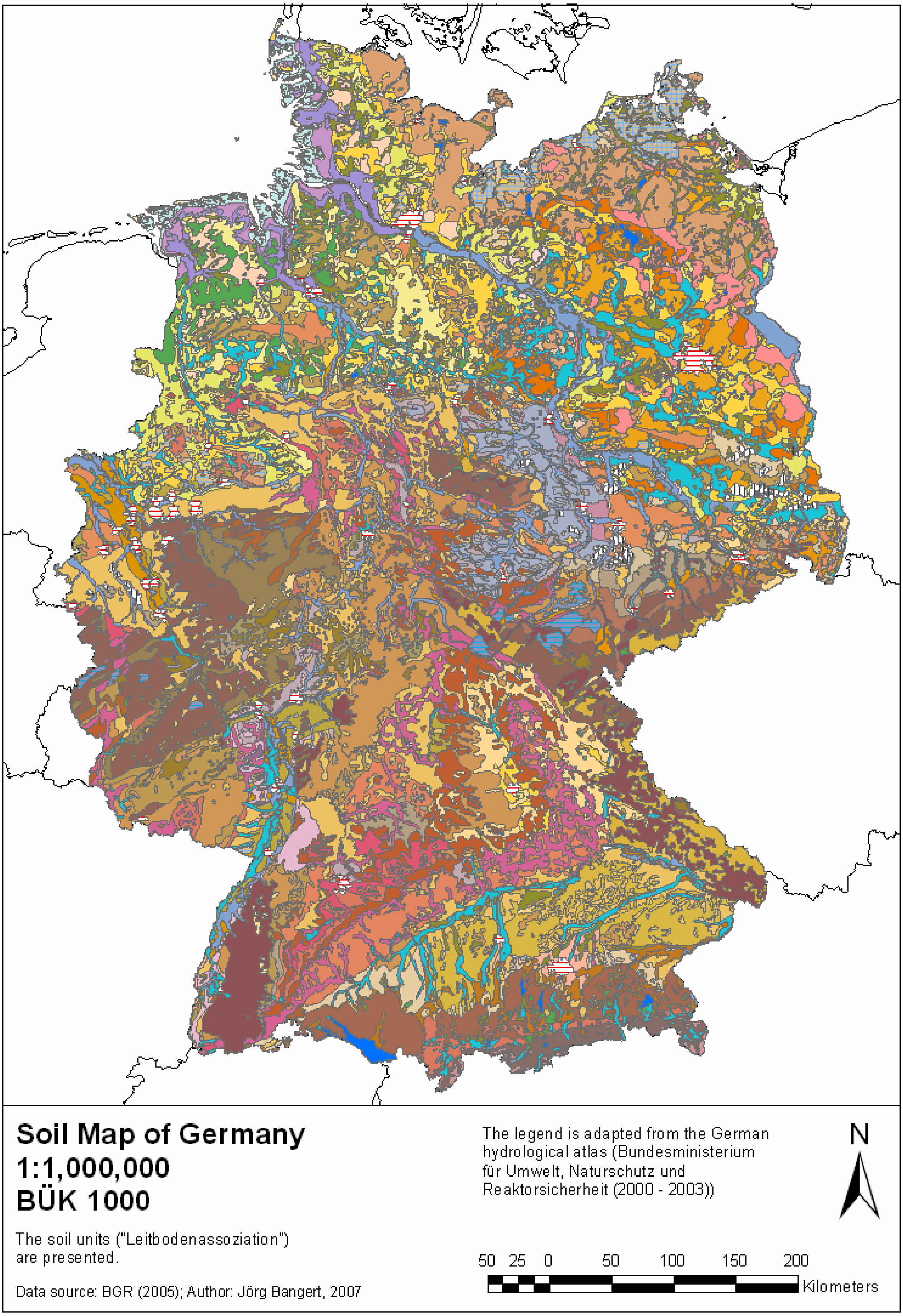


Figure A 6: **Map of the BÜK 1000 of Germany**

Soil Associations with Main Soil Types and Parent Material

Soils of the coastal area and bog soils

1 Dystric Regosols from sand dunes
2 Salo-Thionic Gleysols in the tidal areas of the North Sea
3 Calcaric and Eutric Gleysols from marine sediments (tidal marsh)
4 Eutric Fluvisols from brackish sediments (tidal marsh)
5 Eutric Fluvisols from fluviatile sediments
6 Eutric Histosols
7 Dystric Histosols

Soils of the fluvial plains and lowlands

8 Fluvisols / Gleysols from loamy to clayey fluviatile sediments
9 Gleyic Chernozems from calcareous silty to clayey sediments
10 Fluvisols / Gleysols from sandy to sandy-loamy fluviatile sediments
11 Fluvisols / Gleysols from frequently alternating sandy to clayey fluviatile sediments
12 Gleysols from sandy sediments of the ice-marginal valleys and lowlands
13 Calcaric Regosols / Calcaric Fluvisols from calcareous sandy to loamy sediments of river terraces
14 Haplic Luvisols from silty to loamy periglacial sediments overlying glacial gravels
15 Haplic Luvisols from loess-covered loamy to sandy river-terrace deposits
16 Dystric Cambisols from sandy river-terrace deposits
17 Haplic Podzols / Cambic Podzols / Gleyic Podzols from sandy fluviatile sediments

Soils of the glacial drift area including the Tertiary hills of the Alpine foreland

18 Eutric Cambisols / Haplic Luvisols / Calcaric Regosols from Tertiary loess-bearing sediments
19 Haplic Luvisols / Eutric Podzoluvisols / Stagnic Luvisols from boulder clay
20 Luvic Chernozems / Stagnic Chernozems from boulder clay
21 Eutric Cambisols / Haplic Luvisols / Calcaric Regosols from calcareous loamy to sandy morainic deposits
22 Stagnic Gleysols / Spodic Gleysols from boulder clay with a loamy to sandy cover
23 Stagnic Gleysols from loamy to sandy till
24 Stagnic Chernozems from loamy-sandy sediments overlying boulder clay
25 Spodic Luvisols / Spodic Podzoluvisols from sandy sediments overlying boulder clay
26 Dystric Podzoluvisols / Luvic Arenosols / Dystric Cambisols from sandy sediments overlying boulder clay
27 Calcaric and Umbric Regosols / Luvic Arenosols from sandy to loamy end moraine deposits (alternating patches)
28 Stagnic Cambisols / Stagnic Podzoluvisols from loamy to sandy deposits overlying boulder clay
29 Stagnic Gleysols from sandy deposits overlying boulder clay
30 Eutric Cambisols / Stagnic Gleysols from calcareous loamy and sandy to gravelly morainic deposits mixed with loess
31 Cambic Podzols / Spodic Arenosols from dry dystrophic sand deposits
32 Eutric Cambisols / Luvic Arenosols from eutrophic sand deposits
33 Haplic Podzols / Dystric Regosols from dry dystrophic sand deposits
34 Dystric Regosols from dry dystrophic sand deposits

Legend of the BÜK 1000 Soil Map of Germany 1:1,000,000

Part 1

The soil associations with main soil type and parent material are shown.

The legend is adapted from the German hydrological atlas (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit (2000 - 2003)).

Data source: BGR (2005); Author: Jörg Bangert, 2007

Figure A 7: **Legend of the BÜK 1000 of Germany – part 1**

Soil Associations with Main Soil Types and Parent Material

Soils in loess areas

■	35	Calcaric Regosols / Haplic Chernozems / Eutric Cambisols from loess alternating with Rendzic Leptosols from marlstone and limestone
■	36	Haplic Chernozems from loess overlying boulder clay
■	37	Haplic Chernozems from loess
■	38	Haplic Chernozems / Stagnic Chernozems from loess overlying claystone and marlstone
■	39	Chernozems from loess and loess-like sediments
■	40	Phaeozemic Luvisols / Luvic Phaeozems from loess or loessic loam
■	41	Phaeozemic and Haplic Luvisols from sandy loess overlying sandy glacial sediments or boulder clay
■	42	Haplic Luvisols / Eutric Podzoluvisols / Stagnic Gleysols from various siliceous weathering products mixed with loess
■	43	Stagnic Gleysols from loess or loessic loam overlying various rocks
■	44	Haplic Luvisols / Eutric Podzoluvisols / Stagnic Gleysols from loess or loessic loam overlying various rocks
■	45	Haplic Luvisols / Eutric Podzoluvisols / Eutric Cambisols from loess and loessic loam overlying siliceous weathering products
■	46	Haplic Luvisols / Eutric Podzoluvisols / Eutric Cambisols from sandy loess overlying sand or loam
■	47	Eutric Cambisols / Stagnic Gleysols from loessic loam with fragments of basalt
■	48	Stagnic Gleysols / Eutric Cambisols / Haplic Luvisols from loess or loessic loam

Mountain and hill soils from solid rocks, their weathering products, and redeposited material

■	49	Rendzic Leptosols from slope deposits over limestone, marlstone, and dolomite alternating with Chromic Cambisols and Chromic Luvisols from silty and clayey material derived from limestone weathering
■	50	Eutric and Chromic Cambisols from redeposited material derived from limestone, marlstone, and dolomite weathering and Rendzic Leptosols from limestone
■	51	Vertic Cambisols / Stagnic Gleysols from marlstone and claystone weathering
■	52	Eutric Cambisols from marlstone and calcareous gravels
■	53	Eutric Cambisols from basic and intermediate igneous rocks
■	54	Eutric Cambisols from tuffs rich in bases
■	55	Dystric Cambisols from acid igneous and metamorphic rocks
■	56	Dystric Cambisols / Stagnic Gleysols from weathered metamorphic rocks, sandstone, quartzite, and acid to intermediate igneous rocks
■	57	Spodic Cambisols from acid igneous and metamophic rocks
■	58	Haplic and Spodic Cambisols from siltstone, sandstone, and claystone
■	59	Haplic and Spodic Cambisols from hard argillaceous and silty slates with greywacke, sandstone, quartzite, and phyllite
■	60	Spodic Cambisols from hard argillaceous and silty slates, greywacke, and phyllite
■	61	Dystric Cambisols from quartzitic sandstones and conglomerates with low base status
■	62	Cambisols from loess-bearing sediments overlying sandstone and quartzite
■	63	Cambic and Haplic Podzols from sandstone and quartzite with low base status
▤	64	Stagnic and Spodic Gleysols from loamy and gritty cover sediments mixed with loess overlying sandstone and quartzite
■	65	Frequently alternating Dystric and Spodic Cambisols / Rendzic Leptosols / Haplic Luvisols from slate, greywacke, and limestone, and loessic loam overlying various rocks
■	66	Frequently alternating Rendzic and Umbric Leptosols / Spodic and Vertic Cambisols / Haplic Luvisols /Stagnic Gleysols from limestone and marlstone, sandstone, siltstone and claystone and loessi
■	67	Acrisols / Ferralsols formed during the Tertiary

Alpine soils

■	68	Soils of different altitudes of the Alps from limestone and dolomite (e.g. Rendzic Leptosols / Calcaric Cambisols), and non-calcareous silicate rocks (e.g. Umbric Leptosols / Spodic Cambisols / Stagnic Gleysols)
■	69	Lithic Leptosols of the higher altitude zones of the Alpes

Anthrosols, settlements, and surface water

▤	70	Sealed areas in larger cities (Urbic Anthrosols)
▥	71	Soils redeposited by man and large open-cast mines (Cumulic Anthrosols)
■	72	Surface water

Legend of the BÜK 1000 Soil Map of Germany 1:1,000,000

Data source: BGR (2005); Author: Jörg Bangert, 2007

Part 2

The soil associations with main soil type and parent material are shown.

The legend is adapted from the German hydrological atlas (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit (2000 - 2003)).

Figure A 8: **Legend of the BÜK 1000 of Germany – part 2**

```
*-------------------------------------------------------------------------------
* APPLICATION FILE FOR GEOPEARL
* =============================
*
* File containing the application data for GeoPEARL
*
* Version 1 created by Aaldrik Tiktak in 2003
* ,,> Compatible with GeoPEARL version 1.3.7.
*
* Version 2 created by Aaldrik Tiktak on 15-Jan-2004
* ..> Compatible with GeoPEARL version 1.4.1.
* ..> No changes
*
* Version 3 created by Joerg Bangert on 21-March-2006
*..> for German GeoPEARL_DE
*--------------------------------------------------------------------------------------

*--------------------------------------------------------------------------------------
* Application table takes the following forms:
*
* Column 1: Date
* Column 2: Application type: AppSolSur, AppSolInj, AppSolTil, AppCrpUsr
*
* If Type = AppSolSur (soil surface application):
* Column 3: Dosage (kg/ha) [0|-]
*
* If Type = AppSolInj (injection):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Injection depth (m) [0|-]
*
* If Type = AppSolTil (tillage):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Tillage depth (m) [0|-]
*
* If Type = AppCrp (application to the crop canopy):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Fraction of dosage applied to the crop canopy (-) [0|1]
*-------------------------------------------------------------------------------------

*-------------------------------------------------------------------------------------
* Aplication to the soil surface on 26 May

[springsurface]

1      DelTimEvt            Application frequency

table Applications
26-May  AppSolSur 1
end_table

table TillageDates
end_table

[end_springsurface]

*-------------------------------------------------------------------------------------
```

Figure A 9: Example of an app-file

```
*-------------------------------------------------------------------------------
* COMPOUND FILE FOR GEOPEARL
* ==========================
*
* FILE COMPATIBLE WITH GEOPEARL_1_1_1
*-------------------------------------------------------------------------------

*-------------------------------------------------------------------------------
* Default substance parameters
* These parameters can be overwritten by including them into the compound section
* of the relevant pesticide

*-------------------------------------------------------------------------------
* Gas/liquid partitioning parameters
20.0              TemRefVap  (C)         .. measured at [0|40]
95.0              MolEntVap  (kJ.mol-1)     Molar enthalpy of vaporisation [-200|200]
20.0              TemRefSlb  (C)         .. measured at [0|40]
27.0              MolEntSlb  (kJ.mol-1)     Molar enthalpy of dissolution [-200|200]
0.0               MolEntSor  (kJ.mol-1)     Molar enthalpy of sorption [-100|100]
20.0              TemRefSor  (C)         .. measured at [0|40]

*-------------------------------------------------------------------------------
* Uptake parameters
0.5               FacUpt     (-)         Coefficient for uptake by plant [0|10]

*-------------------------------------------------------------------------------
* Diffusion of solute in liquid and gas phases
4.3d-5            CofDifWatRef (m2.d-1)  Reference diff. coeff. in water [10e-5|3e-4]
0.43              CofDifAirRef (m2.d-1)  Reference diff. coeff. in air [0.1|3]
20.0              TemRefDif  (C)         Diff. coeff measured at temperature [10|30]

*-------------------------------------------------------------------------------
* Transformation rate parameters
20.0              TemRefTra (C)          Temperature at which DT50 is measured [5|30]
0.70              ExpLiqTra (-)          Exponent for the effect of liquid [0|5]
OptimumConditions OptCntLiqTraRef        OptimumConditions or NonOptimumConditions
1.0               CntLiqTraRef (kg.kg-1) Liq. content at which DT50 is measured [0|1]
54.0              MolEntTra (kJ.mol-1)   Molar activation energy [0|200]

*-------------------------------------------------------------------------------
* Sorption parameters
0.9               ExpFre     (-)         Freundlich sorption exponent [0.1|1.3]
1.0               ConLiqRef  (mg.L-1)    Reference conc. in liquid phase [0.1|-]
0.0               pHCorrection    (-)    pH correction [-2|1]

*-------------------------------------------------------------------------------
* Non-equilibrium sorption
0.00              CofDesRat  (d-1)       Desorption rate coefficient [0|0.5]
0.5               FacSorNeqEql (-)       CofFreNeq/CofFreEql [0|-]

*-------------------------------------------------------------------------------------
* Substance specific substance properties.
*-------------------------------------------------------------------------------------
* CMPA = FOCUS compound_A

[CMPA]

table FraPrtDau (mol.mol-1)
end_table

pH-independent   OptCofFre_A                  [pH-dependent|pH-independent|GeoPEARL]
Input            OptDT50_A                    Option for DT50 [Input|Calculate]
300.0            MolMas_A       (g.mol-1)    Molar mass [10|10000]
60.0             DT50Ref_A      (d)          Half-life time [1|1e6]
60.0             KomEql_A       (L.kg-1)     Coef. eql. sorption on org. matter [0|1e9]
1.d-10           PreVapRef_A    (Pa)         Saturated vapour pressure [0|2e5]
90.0             SlbWatRef_A    (mg.L-1)     Solubility in water [1e-9|1e6]
1.d6             DT50DspCrp_A   (d)          Half-life time on crop [1|1e6]
1.d-4            FacWasCrp_A    (m-1)        Washoff factor [1e-9|1e6]

[end_CMPA]
```

Figure A 10: Example of a cmp-file

```
*-------------------------------------------------------------------------------
* UC LIST FILE FOR GEOPEARL
* ============================
*
* File containing the UC ID’s included in the simulation
*
* Version 1 created by Jörg Bangert in 2005
* ,,> Compatible with GeoPEARL version ?.
*
*-------------------------------------------------------------------------------

* Choose between one of the two forms
* The first table describes a range of UC from <first value> to <second value>
* The second table list the UC to be calculated

table PlotList
4720 4869
end_table

*table PlotList
*1
*2
*300
*7744
*end_table
```

Figure A 11: Example of a lis-file

```
*-------------------------------------------------------------------------------
* GeoPearl input file
* This version is compatible with GeoPEARL_1_1_1
* Please make a copy of this file before editing
*
1 ModelVersion  Model version
1 GUIVersion    GUI version
1 DBVersion     Database version
*-------------------------------------------------------------------------------
* GeoPEARL control
*-------------------------------------------------------------------------------
* Directory structure - use either full or relative path names:
* 1. If FULL path names are used, please avoid spaces.
* 2. If RELATIVE names are used, the path is relative to the position of the
*    geopearl.exe file.
..\bin         BinDir                  Binary directory
output         OutputDir               Output directory
..\ger_scheme  SchematisationDir       Spatial schematisation directory
Tmp            PearlDir                Tmp directory for PEARLMODEL

* General control
IOMode_Full     IOMode                  Screen control [IOMode_Full|IOMode_StdOut]
Low             PriorityClass           Priority class [Low|Normal|High]
New             OptAppend               Append results (Yes|No|New|SkipErrors)?
Yes             OptDelPloFiles          Should other files be removed (Yes|No)?

* Timers - TimStart and TimEnd must be in range with dates in .met files
01-Jan-1901     TimStart                Start time of the simulation
31-Dec-1919     TimEnd                  End time of simulation
6               InitYears               Number of years for initialization (0|10)

* Number of CPUs available for grid computing
1               NumCPU                  Number of CPUs (1|-)
1               CPUID                   Number of the current CPU (1|NumCPU)
*-------------------------------------------------------------------------------
* Reference to plot file and plots included in model run
* The plot files must be stored in the schematisation directory
*-------------------------------------------------------------------------------
germany           Plots             Plot file (plo file - in schematisation dir)
Manual            OptPlotList       Option: (Automatic|Manual|Generate_Only)
*-------------------------------------------------------------------------------
* If OptPlotList = Automatic
* Crop area database (unc file) must be stored in the schematisation directory
* For guidelines with respect to the selection of the number of zones:
* please read the manual
Germany         CropAreaDatabase        File with crop area per UC (unc file)
0               ThresholdArea   (ha)    Threshold area (0|-)
7744            NumZone                 Number of zones (2|-)
Rank            OptPlotSelection        Option: (Neighbour|Rank)

* Crops for which a registration is submitted. The model takes the sum of the
* crop areas of the individual crops. Make sure that the name is exactly equal
* to one of the names in the crop area database (unc file)

table Crops
1  winter_cereals
end_table
*-------------------------------------------------------------------------------
* If OptPlotList = Manual
* Specify file with UC ID’s
germany           PlotListFile            File with UC to be included
*-------------------------------------------------------------------------------
* missers - file must be put in schematisation directory
crop              SwapMisFile             File with missers
*-------------------------------------------------------------------------------
* Compound and application information
*-------------------------------------------------------------------------------
germany               CompoundProperties     Compound properties
germany               ApplicationSchemes     Application schemes
*-------------------------------------------------------------------------------
* Substances and application scheme. A run is made for each substance included
* Column 1  : Pesticide code - must be included in CompoundProperties file
* Column 2  : Application code - must be included in Applications file
* Column 3+ : Compound codes included in run (first = the daughter)
```

```
table Runs
CMPA springsurface A
end_table
*-------------------------------------------------------------------------------
* Soil information
* The soil file must be placed in the schematisation directory

germany        SoilDatabase             Soil database (sol file)

*-------------------------------------------------------------------------------
* Crop information
* The crop file must be placed in the schematisation directory

Ger_maize        CropDatabase             File with crop properties (crp file)

*-------------------------------------------------------------------------------
* Information about meteo stations
* The meteo files must be stored in the schematisation directory
* Column 1: ID
* Column 2: Latitude
* Column 3: Altitude (m)
* Column 4: Initial temperature (C)
* Column 5: Option for potential evapotranspiration
* ...       Input          : Reference evapotranspiration provided by user
* ...       Penman         : Penman reference evapotranspiration
* ...       Makkink        : Makkink reference evapotranspiration
* ...       PenmanMonteith : Penman Monteith evapotranspiration
* Column 6: Reference to the meteo file (met file)

table MeteoStations
         1      52.0      10.0      9.97    Input          1
         2      52.0      10.0      9.97    Input          2
         3      52.0      10.0      9.97    Input          3
(…)
      7744      52.0      10.0      9.97    Input       7744
end_table

*-------------------------------------------------------------------------------
* Local and regional groundwater system
* These files must be stored in the schematisation directory
Germany        GroundwaterSystem      Groundwater system (lbo file)
Germany        DrainageSystem         Local drainage system (dra file)
*-------------------------------------------------------------------------------
* Output control data

No           OptScreen           Screen option (No|Swap_Only|Yes)
germany      OutputControl       File with output data (ctr file)
Yes          PrintCumulatives    Print fluxes cumulative (Yes|No)
Fixed        OptZFoc             Option for ZFOC (Fixed|Variable)
1.0          ZFoc          (m)   Depth of layer for balances (0.1|-)
DaysFromSta  DateFormat    Format of dates in the output file (DaysFromSta|DaysFrom1900|Years)
G12.4        RealFormat          Format of reals in the output file (FORTRAN format)
Decade       OptDelTimPrn        Option for time step (Day|Decade|Month|Year|Calculated|Other)
1.0          DelTimPrn (d)       Print time step - only if option is input (1.0|-)
Automatic    OptHyd              SWAP mode: (Automatic|OnLine|Only)
GeoPEARL     OptReport          (FOCUS|DutchRegistration|GeoPEARL) report

*-------------------------------------------------------------------------------
* SWAP control parameters

No                OptHysteresis          Simulate hysteresis (No|Yes)
1000000           MaxItSwa               Maximum number of iterations (2|1000000)
0.005             ThetaTol      (m3.m-3) Tolerance for SWAP (1e-5|1e-2)
1.d-5             DelTimSwaMin  (d)      Minimum time step for SWAP (1e-8|0.1)
0.20              DelTimSwaMax  (d)      Maximum time step for SWAP (0.01|0.5)
1.0               GWLTol        (m)      Tolerance for groundwater level (1e-7|1e2)

*-------------------------------------------------------------------------------
* End of file
```

Figure A 12: Example of a geo-file

Appendix B: Investigation of the scaling factors – statistical tests

By scaling the MARS climate information using the DWD long-term values, the original data were changed. It is necessary to show that the resulting data sets do not represent less conservative weather conditions than the original MARS data. Regarding the mean and the median of the scaling factors for temperature and precipitation (see Table A 2 and Table A 3), differences can be assumed.

Table A 2: Mean and median of the scaling factors for temperature of DWD and MARS data

	Scaling factor
Mean	-1.30
Median	-1.26

Table A 3: Mean and median of the scaling factors for precipitation of DWD and MARS data

	Scaling factor
Mean	1.14
Median	1.09

As the scaling factor for temperature will be added to the data of the MARS data set, the negative mean shows that the MARS values for temperature are reduced by 1.3 °C in average. For the derivation of the precipitation the MARS values are multiplied by the scaling factors, i.e. the precipitation values increases in average. Thus the DWD data set seems to show colder and wetter climate conditions which represent more conservative conditions regarding the leaching behaviour and the degradation rate of the substance. These assumptions were clarified by a statistical test.

Wilcoxon-Test

For each raster cell, long-term monthly values of the MARS data set and of the DWD data set were compared. The data distribution cannot be considered to be normal distributed and the data are dependent. An appropriate test – the Wilcoxon test – was carried out. The test compares pairs of data and analyses if the medians of two samples are significantly different or not. For the test, the 7744 long-term monthly values of the DWD for each scenario were paired with the long-term monthly values of the MARS data (the long-term value of the covering MARS tile was assigned to each scenario). Thus the two medians of the 12 * 7744 = 92928 data pairs were compared for temperature and for precipitation.

Table A 4: Results of the comparison DWD and MARS (Statistika: Wilcoxon test, p= 0.05)

Parameter	Z	p-niveau	Result	N
Precipitation	102.7471	< 0.01	significant differences	92928
Temperature	260.1177	< 0.01	significant differences	92928

The high Z-values show that the medians of the DWD data set and the MARS data set are significantly different. As the median of the DWD data set is smaller for temperature and higher for precipitation, it can be assumed, that the DWD data set represents a more conservative approach, i.e. scaling the MARS data to the DWD data leads to wetter and colder weather conditions.

Appendix C: Output files

The results of the simulations are stored permanently during the calculations in ASCII files. Up to nine output files are available which are shortly presented here.

The wsb-file
- contains the annual and long-term average water balances of the soil profiles.

The wfb-file
- contains the annual and long-term average water balances of the FOCUS layer.

The csb-file
- contains the annual and long-term average substance balances of the soil profile.

The cfb-file
- contains the annual and long-term average substance balances of the FOCUS layer.

The ccb-file
- contains the annual and long-term average substance balances of the crop canopy.

The foc-file
- contains the percentiles of the leaching concentration at target depth.

The day-file
- The day-file is only created if detailed output is requested in the geo-file. In standard applications the file is empty.

The log-file
- The log-file contains the program log. Information on the model run is available, e.g. the calculation time, the UC included in the run, and the used soil data, weather data and application schedule.

The err-file
- The err-file contains error messages. If no error occurs the file is empty or not available.

The crf-file
- The crf-file is created in special application mode of GeoPEARL. The file gives the linkage between the zone number and the UC ID and is required for the creation of output maps (see chapter 8.2.2).

For further information about the output files the user is referred to the GeoPEARL manual (Tiktak et al., 2004a, p. 51). The output data are presented as space separated text in the files. They can be easily transformed into tables and joined to the map-file in a GIS.