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Protect groundwater from plant protection products

Spatial distributed leaching modelling to identify agricultural areas with high risk for leaching

by:

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Abstract: Protect groundwater from plant protection products. Spatial distributed leaching modelling to identify agricultural areas with high risk for leaching

The Federal Environment Agency is responsible for environmental risk assessment in the context of authorisation of plant protection products. The current groundwater exposure assessment at national level is based on the use of a single scenario. However, the harmonised tiered approach for the groundwater assessment in the EU aims to improve the prediction of leaching of plant protection products into groundwater in the future based on the method of spatially distributed leaching modelling (SDLM). Appropriate simulation models that can meet this requirement are currently missing or have not yet been sufficiently validated. The aim of the project was to investigate what adjustments are necessary at national level to ensure adequate and reliable prediction of the leaching potential of active substances and metabolites using the method of SDLM for the agricultural area in Germany. In this context, the implementation of additional processes of the water balance in the unsaturated soil zone in PELMO was investigated. Involving a panel of experts, it was decided to develop a new version of GeoPELMO DE that considers the processes of chromatographic flow (matrix flow), preferential flow (macropore flow), surface runoff and drainage. As a result, it was necessary to extensively review and adapt soil, climate and groundwater data available nationwide. Additional investigations were carried out using lysimeter studies and monitoring data from Denmark for a mean calibration of macropore flow in three soil classes. The influence of the additionally implemented processes on the soil water balance and the prediction of percolate water concentrations was analysed. Runoff and drainage had the greatest influence on the water mass balance. Macropore flow and the parametrisation of the organic carbon content in the subsoils had the greatest impact on the substance concentrations in the leachate. A percentile comparison showed that the results of the nationwide predicted leachate concentrations with GeoPELMO DE are more conservative than the currently used national approach based on the Hamburg scenario for a relatively high proportion of the active substances and metabolites investigated. This finding is independent of whether the FOCUS leaching approach based on matrix flow or an extended approach including runoff, macropore flow and drainage is used. However, the ranking of the FOCUS Hamburg scenario as a percentile of nationwide concentrations is lower when the modelling approach is supplemented by these three processes. This means that, in the lower tier groundwater exposure assessment based on the Hamburg scenario, the use of uncertainty factors would be necessary if higher tier simulations with the GeoPELMO DE model would to be used for regulatory purposes in the future. Such regulatory decisions have complex implications and should finally be based on comprehensive and extensive modelling results. Several alternative scenarios were selected from two model versions of GeoPELMO DE and tested on 11 real active substances and 34 metabolites. From a modelling perspective, it can be concluded that finally only spatial models like GeoPELMO DE are able to equally predict an accurate temporal and spatial percentile for all active substances and metabolites. Individual climate-soil-combinations can serve as an approximation, although in specific cases it must always be expected that there may be deviations from the results of a geo-version of the model. It remains therefore difficult to recommend the use of individual scenarios for different substance properties, crops or PPP application patterns based on the analyses carried out, especially since it was not possible to carry out a nationwide comparison with monitoring data within the framework of the project.

Kurzbeschreibung: Grundwasser vor Pflanzenschutzmitteln schützen. Identifizierung von landwirtschaftlichen Gebieten mit hohem Versickerungsrisiko durch räumliche Modellierung

Das Umweltbundesamt ist im Rahmen der Zulassung von Pflanzenschutzmitteln für die Umweltrisikobewertung zuständig. Die aktuelle Expositionsbewertung Grundwasser auf nationaler Ebene basiert auf der Verwendung eines einzelnen Szenarios. Das in der EU harmonisierte Stufenkonzept für die Grundwasserbewertung sieht jedoch vor, Einträge von Pflanzenschutzmitteln ins Grundwasser zukünftig mit Hilfe räumlicher Modellabschätzungen besser vorhersagen zu können. Entsprechende Simulationsmodelle, welche diese Anforderung erfüllen können, fehlen bislang oder wurden bisher nicht ausreichend validiert. Das Ziel des Projekts war zu untersuchen, welche Anpassungen national erforderlich sind, um eine angemessene und zuverlässige Vorhersage des Versickerungspotenzials von Wirkstoffen und Metaboliten mit der Methode räumlicher Modellierung für die landwirtschaftliche Fläche in Deutschland zu gewährleisten. In diesem Zusammenhang wurde die Implementierung zusätzlicher Prozesse des Wasserhaushalts in der ungesättigten Bodenzone in PELMO untersucht. Unter Einbeziehung eines Expertenrats wurde beschlossen, eine neue Version von GeoPELMO DE zu entwickeln, in der die Prozesse chromatographisches Fließen (Matrixfluss) und präferentielles Fließen (Makroporenfluss) sowie Oberflächenabfluss (Runoff) und Drainage berücksichtigt werden. Infolgedessen war eine umfangreiche Sichtung und Anpassung bundesweit verfügbarer Boden-, Klima- und Grundwasserdaten notwendig. Zusätzliche Untersuchungen wurden anhand von Lysimeterstudien und Monitoringdaten aus Dänemark für eine mittlere Kalibrierung des Makroporenflusses in drei Bodenklassen durchgeführt. Der Einfluss der zusätzlich implementierten Prozesse auf den Bodenwasserhaushalt und die Vorhersage von Sickerwasserkonzentrationen wurden analysiert. Runoff und Drainage zeigten den größten Einfluss auf den Wasserhaushalt. Der Makroporenfluss und die Parametrisierung des organischen Kohlenstoffgehalts in den Unterböden hatten die größten Auswirkungen auf die Stoffkonzentrationen im Sickerwasser. Ein Perzentil-Vergleich zeigte, dass die Ergebnisse der bundesweit vorhergesagten Sickerwasserkonzentrationen mit GeoPELMO DE für einen relativ hohen Anteil der untersuchten Wirkstoffe und Metaboliten konservativer sind als der derzeit verwendete nationale Ansatz auf Basis des Hamburg-Szenarios. Diese Erkenntnis ist unabhängig davon, ob der FOCUS-Versickerungsansatz mit Matrixfluss oder ein erweiterter Ansatz inklusive Oberflächenabfluss, Makroporenfluss und Drainage verwendet wird. Die Rangfolge des FOCUS-Hamburg-Szenarios als Perzentil der bundesweiten Konzentrationen fällt jedoch geringer aus, wenn der Modellierungsansatz um die drei Prozesse ergänzt wird. Das bedeutet, dass in der niedrigstufigen Expositionsbewertung Grundwasser anhand des Hamburg-Szenarios die Verwendung von Unsicherheitsfaktoren erforderlich wäre, wenn zukünftig höherstufige Simulationen mit dem Modell GeoPELMO DE regulatorisch verwendet werden sollen. Solche regulatorischen Entscheidungen haben komplexe Auswirkungen und sollten letztlich auf umfassenden und umfangreichen Modellierungsergebnissen basieren. Aus zwei Modellversionen von GeoPELMO DE wurden mehrere alternative Szenarien ausgewählt und an realen 11 Wirkstoffen und 34 Metaboliten getestet. Aus modelltechnischer Sicht lässt sich schlussfolgern, dass nur räumliche Modelle wie GeoPELMO DE in der Lage sind, ein exaktes zeitliches und räumliches Perzentil für alle Wirkstoffe und Metaboliten gleichermaßen vorherzusagen. Einzelne Klima-Boden-Kombinationen können als Annäherung verwendet werden, wobei im konkreten Fall immer damit gerechnet werden muss, dass es zu Abweichungen von den Ergebnissen einer Geo-Version des Modells kommen kann. Es bleibt daher schwierig, anhand der durchgeführten Analysen die Verwendung einzelner Szenarien für unterschiedliche Stoffeigenschaften, Kulturen oder PSM-Anwendungsmuster zu empfehlen, zumal ein bundesweiter Abgleich mit Monitoringdaten im Rahmen des Projektes nicht realisiert werden konnte.

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List of abbreviations

Abbreviation	Meaning
AKTIS	Amtliches Topographisch-Kartographisches Informationssystem (Official Topographic-Cartographic Information System)
APECOP	Project name: Effective approaches for Assessing the Predicted Environmental Concentrations of Pesticides
ArcEGMO	ArcEGMO Hydrological catchment modelling system with GIS integration (ArcGIS-based catchment model)
BB	Brandenburg
BBA	Biologische Bundesanstalt für Land- und Forstwirtschaft
BBCH	Biologische Bundesanstalt, Bundessortenamt und Chemische Industrie (Skala für Pflanzenentwicklungsstadien)
BGR	Bundesanstalt für Geowissenschaften und Rohstoffe
BK50	Bodenkarte 1:50.000 (Soil map 1:50,000))
BKA	Bodenkundliche Kartieranleitung (Soil mapping instructions)
BÜK200	Bodenübersichtskarte Deutschlands 1:200.000 (Soil overview map of Germany 1:200,000)
BÜK250	Bodenübersichtskarte Deutschlands 1:250.000 (Soil overview map of Germany 1:250,000)
BÜK1000N	Nutzungsdifferenzierte Bodenübersichtskarte Deutschlands 1:1.000.000 (Land use differentiated Soil overview map of Germany 1:1,000,000)
CREAMS	Field Scale Model for Chemicals/ Runoff, and Erosion from Agricultural Management Systems (Knisel 1980)
C_{org}	Organic Carbon
$DegT_{50}$	Time to reach 50% of degradation
DOC	Dissolved Organic Carbon
DWA	Deutsche Vereinigung für Wasserwirtschaft, Abwasser und Abfall e. V. (German association for water, wastewater and waste management)
DWD	Deutscher Wetterdienst (German weather service)
EC	European Commission
EU	European Union
FC	Field Capacity in soil
f_{eff}	Drainagesystem efficiency factor
FHG	FOOTPRINT Hydrologic Soilgroup
FOCUS	FOrum for the Co-ordination of pesticide fate models and their USe
FOCUS PEARL	FOCUS model PEARL
FOCUS PELMO	FOCUS model PELMO
FOCUS MACRO	FOCUS model MACRO
FOCUS L	Leaching model version of GeoPELMO DE considering chromatigraphic (matrix) flow

Abbreviation	Meaning
FOCUS L+R+M+D	Leaching model version of GeoPELMO DE considering chromatigraphic (matrix) flow, Runoff, preferential (Macropore) flow and Drainage
FST	FOOTPRINT soil types
GeoPEARL NL	Geographical version of PEARL considering data from The Netherlands
GEUS	Geological Survey of Denmark and Greenland
GIS	Geographic Information System
GISPELMO	GIS version of PELMO
GLEAMS	Groundwater Loading Effects of Agricultural Management Systems
GUS	Groundwater Ubiquity Score
HAD	Hydrologischer Atlas Deutschland (hydrological atlas Germany)
HÜK	Hydrogeologische Übersichtskarte (hydrogeological overview map)
Kc	Crop coefficient (plant factor for evapotranspiration)
K_{foc}	Sorption constant in soil related to organic carbon (L/kg)
Ksat	saturated hydraulic conductivity in soil
LOD	Limit Of Detection
M1, M2	Dummy metabolites M1, M2
MARS	Managing Aquatic ecosystems and water resources under multiple stress
MACRO	MACRO is a physically based one-dimensional numerical model of water flow and reactive solute transport in field soils
ME	Moisture Equivalent
MNGW/MHGW	Mean lowest/mean highest groundwater level below surface
MV	Mecklenburg-Vorpommern (Mecklenburg-Western Pomerania)
n.a.	Not available
NI	Niedersachsen (Lower Saxony)
NW	Nordrhein-Westphalen (North Rhine-Westphalia)
OC	Organic Carbon
P1, P2, P3	Dummy active (parent) substances P1, P2, P3
PEARL	Pesticide Emission Assessment at the Regional and Local scale
PEC	Predicted Environmental Concentration
PECgw	Predicted Environmental Concentration in groundwater
PELMO	Pesticide LEaching MOdel
pF	Soil water tention
PLAP	Pesticide Leaching Assessment Programme
PPP	Plant Protection Product
PRZM	Pestizide Root Zone Model
PRZM SHG	Hydrologic Soil Group based on PRZM
PSM	Pflanzenschutzmittel (Plant Protection Products)

Abbreviation	**Meaning**
PUF	Plant Uptake Factor
RCN	Runoff Curve Number approach
SH	Schleswig-Holstein
SN	Sachsen (Saxony)
ST	Sachsen-Anhalt (Saxony-Anhalt)
SHG	Soil Hydogical Group
TÜK200	Topographische Übersichtskarte von Deutschland 1:200.000 (Topographical Overview Map of Germany 1:200,000)
UBA	Umweltbundesamt (Federal Environment Agency)
WP	Wilting Point in soil

Summary

Background and objectives

According to Article 4 of the EU Regulation (EC) No. 1107/2009 the Federal Environment Agency (UBA) is responsible for environmental risk assessment for the authorisation of plant protection products (PPP) in Germany and for the approval of active substances in the EU. Essential harmonisation in the groundwater exposure assessment was implemented in Europe since 2014 based on the FOCUS tiered approach. This applies particularly for the assessment in tier 1 and tier 2, where the harmonised FOCUS models PELMO, PEARL and MACRO are used to estimate the leaching behaviour of active substances and metabolites based on chromatographic (matrix) flow in the unsaturated soil zone.

Since 2012 the one-dimensional simulation model FOCUS PELMO in combination with the FOCUS Hamburg scenario is mainly used in Germany to evaluate the leaching potential of active substances and their metabolites for groundwater. This status quo in the national groundwater risk assessment leads back to expert judgement decisions in 1990 and follows the assumption that a sandy soil with low organic carbon content and an Atlantic influenced climate with relatively high precipitation in the winter represents a sufficiently conservative (realistic worst-case) soil-climate combination for estimating the leaching behaviour of active substances and their metabolites from PPPs in agricultural areas in Germany.

An extrapolation of the standard scenario-based FOCUS groundwater models to spatial distributed leaching models and their use for regulatory decision-making in future is currently discussed in the scientific und regulatory community in Europe. This new generation of models is intended to define new scenarios as refinement option as well as to identify vulnerable sites for targeted groundwater monitoring studies. These planned adjustments and developments raise the question of the extent to which additional water transport processes in the unsaturated soil zone, such as preferential flow, runoff, interflow and drainage, as well as sorption in subsoils, should be integrated into existing FOCUS models to ensure reliable prediction of pesticide leaching. For example, EFSA has already criticised the fact that agricultural used areas with soils prone to macropores are unlikely to be covered by the existing FOCUS models and scenarios.

The aim of the project was to determine what adjustments are required in future national groundwater risk assessments for PPPs to ensure an appropriate and reliable prediction of the leaching potential of active substances and their metabolites with the method of spatially distributed modelling. The calibration and implementation of additional processes for the water balance and PPP transport in the unsaturated soil zone in PELMO, e.g. preferential flow, runoff, interflow and drainage, as well as sorption in subsoils, are discussed in the report. The accessibility and quality of national geodata have being evaluated with the aim of extrapolating modelling routines for those processes to different soil and climate conditions in Germany. The extent to which the groundwater exposure assessment is influenced when other processes such as runoff, preferential flow and drainage are considered beside matrix flow has been investigated. New scenarios were selected and analysed to provide recommendations for potential adjustments to the national groundwater modelling approach.

State of knowledge according to runoff, macropore flow, interflow and drainage

A literature review was conducted to answer the question to which extent the soil water processes such as runoff, preferential flow, interflow and drainage, which are currently not considered in national modelling of pesticide leaching into groundwater, are relevant for the water and mass balance in the unsaturated zone under existing soil and climate conditions in Germany.

Since 2000, surface water runoff has been technically considered as an optional modelling routine for the soil water balance in the FOCUS leaching models PELMO and PRZM. Runoff was already considered in an earlier research project for the development of a nationwide groundwater modelling tool for Germany. To implement a modelling routine, the curve number approach based on the FOOTPRINT soil type classification was used, which was originally developed on national level for surface water model called GERDA (GEobased Run-off, erosion and Drainage risk Assessment for Germany). The use of a German soil map with larger scale required further development of the available curve-number approach in the current project.

Preferential flow or macropore flow in soil and the unsaturated zone is a process whose significance has been subject of intensive scientific research at national and international level for many years. Shrinkage cracks in cohesive soils, bio-pores by earthworms, but also differences in the structure of the unsaturated zone referred to lithology or vertically aligned inhomogeneities of the substrate, as well as fractured media like fractured glacier clayey tills, limestone and solid rocks are cited as factors for hydraulic active discontinuities influencing the water balance and the flow and transport of chemicals in subsoils. Long term targeted groundwater monitoring data from the Danish Pesticide Leaching Assessment Programme (PLAP) provide evidence that leaching behaviour of pesticides is influenced by preferential flow depending on soil types, the water balance of the field, including climate, as well time and dose of application. In clayey and silty soils in particular, preferential water flow can contribute to a greater extent to the leaching of PPPs. Related to the characteristic of soils in Germany it can be assumed that a considerable proportion of agricultural soils are potentially affected by preferential flow pattern. Discussions with the experts on the project advisory board revealed that it is difficult to consider all causes of preferential flow and their spatial and temporal characteristics into account in a scientific sound classification, as scientific knowledge and nationwide information and geodata are sometimes unavailable. However, there was also consensus that a lack of scientific information or geodata should not lead to preferential flow being disregarded in the development of spatially distributed models, as this could even lead to higher underestimation of pesticide leaching for certain areas under certain weather conditions. The experts recommended developing a simple soil classification for the implementation of a new modelling routine for macropore flow and calibrating it based on available lysimeter data and monitoring data from the Danish PLAP system.

There are various hydrological concepts relating to interflow or hypodermic flow. In a general understanding, this refers to a rapid access of seeped precipitation water to surface waters in significantly shorter time than via base flow. As part of the project, experts discussed that fast interflow via perched (intermitted) groundwater is a phenomenon that is rather limited in terms of space and time. Subsurface interflow as rapid lateral transport in the subsurface above the groundwater body hardly ever occurs, except in areas with steep slopes in combination with vicinity to surface water bodies. The generation of these lateral natural discharges in the riparian zone are temporally limited to water saturated subsurface soils. Due to the low spatial relevance of the interflow in relation to the agricultural area in Germany and the difficulty of implementing it in a one-dimensional groundwater model, it was decided not to consider interflow as process for modelling pesticide leaching at the national scale.

Drainage as fast subterranean flow via artificial drainpipes into surface waters can appear after precipitation events or during period with rising groundwater levels. Artificial drainage installations are partially known to be widespread in Germany, especially in the northern lowlands. The maps of drainage systems currently available for some federal states are largely based only on potentially existing drainage systems. Any drainage approach that is technically feasible in PELMO can only be developed on the basis percolate water rates, as there is currently no reliable information available about groundwater tables and their seasonal fluctuations in drained areas.

Since sorption on soil organic carbon is one of the most sensitive parameters for the prediction of pesticide leaching, an evaluation of actual measured levels of organic carbon in agricultural soils in Germany, especially in subsoils, is required and was therefore included in the investigations.

Implementation of new processes and soil-climate scenarios in GeoPELMO DE

It was decided during the project to develop a new version of GeoPELMO DE for the agricultural area in Germany considering actual geodata. To parametrize the water balance and pesticide transport in the unsaturated zone down to a soil depth of 1 m, nationwide available soil data on a scale of 1:250.000 was used and adjusted as necessary. The GeoPELMO DE version from a previous project was still based on soil data with a scale of 1:1.000.000, so a comparison of both soil maps was conducted regarding depth dependent organic carbon contents. A statistical analysis of nationwide available measured organic carbon contents provided evidence to replace data from humus class ´0´ with default values of 0.2 % in 0 to 60 cm or 0.1 % in 60 to 100 cm soil depth, both values corresponding to the 30th percentile of measured data for humus class ´0´.

Information from 299 weather stations of the National Meteorological Service in Germany (DWD) was considered for the implementation of climate data. The prerequisite was that a weather station had daily data for air temperature, relative humidity and precipitation as well as partly on evapotranspiration for the period 1985 - 2010. The spatial assignment of the selected weather station data to the German agricultural area is based on a statistical analysis with raster datasets from the DWD with monthly average values of temperature and precipitation for the climate period 1980 – 2009 and a spatial resolution of 1 x 1 km. Finally, a raster dataset of daily weather data with a resolution of 200 x 200 m was developed to match the resolution of the soil map.

To adapt the modelling routine for surface runoff in PELMO, the curve number approach based on the FOOTPRINT soil type classification was applied to all soil profiles of the German soil map with a scale 1:250.000 by assigning them to a corresponding PRZM Hydrologic Soil Group (SHG). The applied methodology is based on a decision tree with several questions, which had to be answered for every soil profile. As the result of this classification, 37.8 % of the German arable land is classified as SHG A, which rather represents permeable soils on sandy and gravelly substrates and is frequently found in Northern Germany. Furthermore, 23.7 % of agriculture fields are classified as SHG B, 27.5 % as SHG B-C and 11.0 % as SHG C, which are characterised by different soil textures and where the tendency for surface runoff more or less increases during heavy rainfall events.

A soil macropore classification was developed which considers the texture and very high humus contents of the soils as well as the local occurrence of groundwater tables very close to the surface. The classification mainly represents the vulnerability of soils to develop and preserve desiccation cracks under dry weather conditions. The tendency of the soils to conserve biopores over time is partially covered by this classification. It was decided to develop three vulnerability classes and to apply the macropore classification to a soil profile depth of 1 m. Approximately 12.3 % of the German crop land is classified as having a tendency for high macropore flow, 52.9 % susceptible to moderate macropore flow and 34.8 % as not susceptible to macropore flow. The latter are highly permeable sandy soils which mainly occur in Northern Germany. In PELMO, a static and a dynamic modelling approach were developed to parametrise macropore flow beside matrix flow. Both the static and the dynamic approach were tested in comparison with the standard FOCUS modelling routine in PELMO as well as considering an increased dispersion length. To calibrate a suitable depth of the macropore domain and the percentage of macropore flow, long-term drainage data from the PLAP sites Estrup and Silstrup were used for several active substances and their metabolites for a site-specific modelling analysis. The comparative analysis provided evidence that preferential flow occurred during the PLAP and lysimeter experiments on non-sandy soils. It was also observed that the two FOCUS-based model routines in PELMO which are based on matrix flow with standardised and increased dispersion length, were in most cases unable to cover the experimental data, particularly regarding the height and temporal breakthrough of the measured compounds. The measured leaching from the various experiments were best represented by different parameterisations of the proportions of static and dynamic macropore flow. However, it was difficult to find an exact percentage parameterisation of macropore flow that applies to all monitoring and lysimeter results investigated. Finally, the monitoring results for axostrystrobin and its metabolite CyPM from PLAP, as well as the lysimeter results for isoproturon and terbuthylazine, were used to define a low to medium parameterisation of the static and dynamic macropore flow in GeoPELMO DE. Considering the soil classification, 12.3 % of the agricultural soils classified as having a tendency towards high macropore flow are parametrised with a minimum static macropore flow of 4 % and a dynamic macropore flow of up to a maximum of 8 % depending on the site-specific weather conditions. 52.9 % of the agricultural soils classified as having a tendency towards moderate macropore flow are parametrised with 2 % static macropore flow and a dynamic macropore flow fraction up to a maximum of 4 %. No macropore flow is considered for the remaining 34.8 % of the agricultural area in Germany. The trigger for calculating macropore flow with the minimum static percentage in PELMO is a daily precipitation of 10 mm. Depending on the soil moisture content in the preceding 7 days, the dynamic portion of the macropore flow can be higher than the static portion.

To consider the process drainage via artificial drainpipes in GeoPELMO DE, it was decided to focus on potentially drained agricultural areas in Northern Germany, because drainage via tile drains is expected to be more important in the northern German lowland, and relevant geodata were available to a higher extent in northern federal states. Available information was used to define potentially drained agricultural areas in seven federal states in Northern Germany. A descriptive statistical evaluation of potentially drained agricultural areas in Schleswig-Holstein, Mecklenburg-West Pomerania, Brandenburg, Saxony-Anhalt, Saxony, Lower Saxony and North Rhine-Westphalia was performed in relation to soil type classes from soil map 1:250.000 to define potentially drained soil types also in Brandenburg, where drainage data were not applicable. A simple drainage efficiency factor (f_{eff}) was developed and evaluated in order to calculate drainage fluxes via drainpipes based on percolate amounts from the unsaturated soil zone with the one-dimensional model PELMO. Mean drainage rates were obtained for several soil type classes from the soil map 1:250.000. Corresponding spatial data have been made available from three federal states in Northern Germany: Mecklenburg-West Pomerania, Lower Saxony and Saxony-Anhalt. The different drainage rates derived for the soil types were used in GeoPELMO DE as drainage efficiency factors (f_{eff}) for all drained scenarios. Since no spatial information is available about the depth of existing artificial drainage systems and fluctuating groundwater tables in Northern Germany, a standard soil depth of 80 cm was defined in PELMO to calculate the loss of drainage fluxes based on simulated percolate amounts. The assumption behind is that drainpipes are always installed at a soil depth above the frequently occurring groundwater level, which can vary at different sites. However, since in the regulatory context the calculated percolate concentration at a soil depth of 1 m is used as an approximate value for estimating groundwater contamination, a compromise had to be found in the model to represent drainage losses at a depth less than 1 m. Modelling results with PELMO indicate that seasonal effects can be observed, with higher drain fluxes modelled in autumn and winter compared to spring and summer.

Spatially distributed modelling results

The new version of GeoPELMO DE was tested for three fictive active substances (P1-P3) and two fictive transformation products (M1, M2) with different degradation rates and sorption values and applications in maize and winter cereals. Four simulation steps were sequentially performed considering matrix flow (1), matrix flow +runoff (2), matrix flow + runoff + macropore flow (3) and matrix flow + runoff + macropore flow + drainage (4) to analyse the influence of each new soil water process on a nationwide scale. As a fifth step, two different default values for the organic carbon content were tested for humus class ‘0’ in the subsoils.

Nationwide results of the simulated soil water regime have been analysed in terms of the influence of individual soil water processes. It was observed, for example, that only runoff slightly reduces evapotranspiration, while other processes such as preferential flow and drainage have no influence on evapotranspiration, because their influence on the soil moisture content of the upper soil layers in PELMO is very limited. Runoff amounts are reduced by maximum of 10 % when macropore flow is considered in the simulation. The effect is relatively small, and the crops evaluated have no significant influence on the reduction of surface runoff. The simulated drainage water volumes depend mainly on the season, with autumn and winter volumes being about three times higher than in the spring and summer. The influence of individual soil water processes on percolate amounts is very different. When runoff is considered, lower percolate volumes are simulated, whereat the impact of the process on annual percolate amounts is rather limited. Only minor differences in surface runoff have been observed between, both crops, maize and winter cereals. The influence of macropore flow on the total amount of percolate is negligible in both crops, with differences of around 1 % of the annual percolate volumes calculated. In comparison, drainage water flow has a larger influence on the annual percolate water volume. Lower percolate volumes are simulated when drainage is considered. However, this influence varies on a nationwide scale, because only a certain proportion of the agricultural area in GeoPELMO DE is potentially drained. Percolate volumes calculated with GeoPELMO DE based on the FOCUS modelling approach (matrix flow only) are of the same order of magnitude as percolate amounts specified in the German Hydrological Atlas. Spatial deviations between the two different approaches are equally distributed and are mainly in the order of up to +/-50 mm per year but can also be higher in individual regions. The additional consideration of the three processes runoff, macropore flow and drainage flow significantly reduces the calculated percolate volumes overall, although the influence macropore flow is rather negligible. This is also reflected in the deviations from the percolate volumes in the Hydrological Atlas.

The distribution of nationwide percolate concentrations for active substances and metabolites modelled with GeoPELMO DE depends on several conditions: the consideration of runoff, macropore flow, drainage flow and their parametrisation, compound properties such as sorption and degradation, PPP application times and crops, as well as the choice of the spatial and temporal percentile. For active substances, considering runoff and drainage mainly led to reduced leachate concentrations in 1 m soil depth. Considering macropore flow generally led to higher concentrations, with the influence of macropore flow itself being higher than different parametrisations of macropore flow. The relative effect of runoff and macropore flow was typically higher for spring application in maize compared to autumn application in winter cereals, with both processes affecting the leachate concentrations in opposite directions. The influence of drainage was generally rather limited, with minor differences observed between the two modelled crops and application times. Since there are seasonal effects of drainwater flow, the influence of drainage on reducing leachate concentrations might be slightly higher in autumn and winter applications. When runoff, macropore flow and drainage were considered together in the modelling routine, higher spatial median and 80th percentile percolate concentrations have been calculated for active substances in most cases compared to the standard FOCUS approach. However, there was also one situation (P1 as mobile, fast degrading substance in winter cereals), in which lower leachate concentrations were calculated. Predicted leachate concentrations based on the FOCUS modelling routine (matrix flow only) are mainly higher in the northern belt in Germany, where glacial deposits and sandy soils are common. Increasing concentrations were predicted in large parts in central and southern Germany when runoff, macropore flow and drainage were additionally included in the modelling. Because of the additional consideration of these three processes, the relative spatial vulnerability of active substances predicted with GeoPELMO DE can change for large areas.

It was observed that the influence of additional processes on the estimated leachate concentrations was significantly lower for metabolites compared to active substances. Runoff, macropore flow and drainage led to both reduced or increased metabolite percolate concentrations. It appears that increasing concentrations due to runoff were found when the parent compound was applied in autumn (winter cereals) and decreasing concentrations were found when the parent compound was applied in spring (maize). Regarding macropore flow or drainage, it is rather difficult to describe the relationship between increasing or decreasing percolate concentrations as a function of various conditions. This is also due to the very low relative changes in metabolite percolate concentrations because of taking these two processes into account. Finally, slightly lower spatial median and 80th percentile percolate concentrations were estimated for metabolites in spring and summer applications when runoff, macropore flow and drainage were considered together in the FOCUS modelling routine in PELMO. In contrast, slightly higher spatial median and 80th percentile leachate concentrations were estimated for the fictive metabolites for applications in autumn and winter when those processes were modelled together. Both slightly increasing and slightly decreasing trends for metabolite seem to be mainly driven by concentration changes due to runoff.

The spatial modelling results are sensitive to the organic carbon content in soil. Replacing humus class ‘0’ with slightly modified default values for organic carbon content led to relatively high changes in leachate concentrations for active substances and metabolites, which occurred largely independently of crops, application times and spatial percentiles. However, the effect is significantly lower for metabolites than for active substances. It is therefore recommended to parametrise organic carbon contents in subsoils as far as possible based on measured values.

Setting the Hamburg scenario into context of nationwide results

An analysis was carried out to determine the level of protection provided by the FOCUS Hamburg scenario, which is currently used in the national groundwater exposure assessment for PPPs, in comparison with cumulative modelling results from GeoPELMO DE for the entire agricultural area in Germany. It could be expected that the percolate concentration predicted from the Hamburg scenario would represent a relatively high percentile compared nationwide modelling results. Covering approximately 80 % of the spatially distributed results would be consistent with the FOCUS concept, according to which the Hamburg scenario represents realistic worst-case climate-soil-conditions in Germany. Based on calculations for few fictive and more realistic pesticide uses, the FOCUS Hamburg scenario did not cover the 80 % of nationwide percolate concentrations in most cases. If the FOCUS leaching concept of chromatographic (matrix) flow was considered in GeoPELMO DE (model version FOCUS L), the leachate concentrations determined with Hamburg for six dummy active substance situations are between 52 % and 70 % (arithmetic mean: 61 %) and for 11 real active substances have been between 58 % and 80 % (arithmetic mean: 69 %) and for 34 real metabolites between 38 % and 80 % (arithmetic mean: 61 %). This means that, for many evaluated compounds, the Hamburg scenario did not reach the 80th percentile compared to the FOCUS L model version. The inclusion of runoff, macropore flow and drainage in addition to the FOCUS modelling routine (model version FOCUS L+R+M+D) resulted in a lower ranking of the Hamburg scenario for active substances and metabolites and a more central spatial percentile compared to nationwide results. Percolate concentrations from the FOCUS Hamburg scenario represented a wider range for six dummy active substance situations between 25 % and 66 % (arithmetic mean: 46 %), for 11 real active substances between 20 % and 80 % (arithmetic mean: 46 %), for eight dummy metabolite situations between 53 % and 80 % (arithmetic mean: 67 %) and for 34 real metabolites between 18 % and 79 % (arithmetic mean: 50 %). The arithmetic mean values for real transformation products were lower compared to dummy metabolites presumably because secondary, tertiary and quaternary metabolites were considered in the real degradation schemes, too. It can be finally concluded that the results from spatially distributed leaching modelling with GeoPELMO DE are more conservative as the currently used national groundwater risk assessment approach for a relatively high proportion of active substances and their metabolites investigated. This finding is independent of whether the FOCUS leaching approach with chromatographic flow or an extended approach with additional processes such as runoff, macropore flow and drainage is used. However, the percentile ranking of the FOCUS Hamburg scenario is lower when the modelling approach is supplemented with runoff, macropore flow and drainage. A further analysis was carried out to investigate the contribution of individual processes to these results.

Recommendations for the national groundwater risk assessment

Alternative scenarios were selected from the two model versions FOCUS L and FOCUS L+R+M+D from GeoPELMO DE that better represent the 80th spatial percentile of national climate-soil conditions than the FOCUS Hamburg scenario. The principle chosen was to identify climate-soil combinations in GeoPELMO DE based on the highest possible number of overlaps between the 75th and 85th spatial percentile from 14 percolate concentration maps (three dummy active substances and four metabolites in two crops). These scenarios were also tested for real active substances and metabolites. The two climate-soil-combinations 6739/2804/Barsinghausen-Hohenbostel and 6126/2620/Hohwacht can be recommended as alternative scenarios for the FOCUS leaching approach (FOCUS L). Both scenarios achieved the 80 ± 5th spatial percentile for most of the dummy active substances and dummy transformation products. In few situations, the estimated leaching concentrations were above the 85th or below the 75th percentile. When comparing the two scenarios with nationwide results for active substances from real pesticide uses, the spatial coverage was between 63 % and 85 % for 6739/2804/Barsinghausen-Hohenbostel and between 73 % and 88 % for 6126/2620/Hohwacht, largely independent of the properties of the substances. The situation is somewhat different for real metabolites. The metabolite concentrations simulated for 6739/2804/Barsinghausen-Hohenbostel ranged between 40 % and 93 % and for 6126/2620/Hohwacht between 43 % and 93 %. These results show that in both scenarios, the level of protection was not achieved for all tested real metabolite situations. However, the calculation of leachate concentrations for metabolites is generally connected to higher uncertainties. Therefore, the results for both scenarios still appear to be acceptable also for transformation products.

The six climate-soil-combinations 6135/2620/Hohwacht, 3162/798/Ulm, 7344/2352/Bad Harzburg, 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig were selected in different steps from the FOCUS L-R+M+D model version, considering chromatographic and preferential flow, runoff and drainage. The extent to which they finally cover the 80 ± 5th spatial percentile for all dummy active substances and dummy transformation products depends on the number of overlaps from the selection step. When comparing the six alternative scenarios with the nationwide results for active substances from real pesticide uses, it was found that the concentrations simulated for 6135/2620/Hohwacht, 3162/798/Ulm and 7344/2352/Bad Harzburg suitable represent the concentrations of the 80th spatial percentile obtained with GeoPELMO DE. In contrast, the results for 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig were more heterogeneous and less protective for active substances. For real metabolites, the situation has proven to be more heterogeneous overall. Nevertheless, the scenarios 3162/798/Ulm and 6135/2620/Hohwacht predominantly represent approximately the 80th spatial percentile of nationwide percolate concentrations for metabolites. In contrast, the results for 7344/2352/Bad Harzburg, 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig are less protective for several real metabolite situations. Of the four scenarios, balanced leachate concentrations could not be derived for all tested real metabolites, particularly from scenarios 69854/10464/Burgwald-Bottendorf and 1945/570/Schleswig, although they represented a better situation for all the dummy metabolites. Based on these results, both 6135/2620/Hohwacht and 3162/798/Ulm and with limitations 7344/2352/Bad Harzburg are recommended as most suitable alternative scenarios, which, compared to the results of GeoPELMO DE (FOCUS L+R+M+D), led to most stable modelling results for active substances and metabolites. However, it must be noted that there is no guarantee that these three individual scenarios will cover a spatial protection level of 80 % for all possible pesticide uses occurring within the regulatory framework.

Independent on the selected scenario, it was found that calculations using one climate-soil-combination for the active substance and subsequent metabolites within one degradation scheme repeatedly produced a wide range of percentiles. This means that a single scenario can hardly be used to guarantee a realistic worst-case situation for all substances of a given degradation scheme. The 80th spatial percentile in a model like GeoPELMO DE would always be represented by different individual climate-soil-combinations for the active substance and various metabolites in one degradation scheme. This result was found to be independent from the model version FOCUS L or FOCUS L+R+M+D. However, the results were more heterogeneous when additional processes such as runoff, preferential flow and drainage were included in the modelling to estimate leachate concentrations.

From a modelling perspective, it can be concluded that finally only a spatial model such as GeoPELMO DE would be able to calculate an exact temporal and spatial 80th percentile for all active substances and metabolites, independent of their properties, their position in the degradation scheme and independent of application pattern of the PPPs. The use of a single scenario can serve as an approximation, but in specific cases would always lead to deviations from the results of a geo-version of the model. It therefore remains difficult to recommend the use of individual scenarios for different substance properties, crops or PPP application patterns. Furthermore, a comparison of nationwide results with GeoPELMO DE and results from the FOCUS Hamburg scenario indicated that uncertainty factors would be necessary for the assessment active substance and metabolites if simulations are performed using the Hamburg scenario currently in use. Such regulatory decisions should finally be based on comprehensive and extensive modelling results.

Zusammenfassung

Hintergrund und Ziele

Das Umweltbundesamt (UBA) ist für die Umweltrisikobewertung in Bezug auf Artikel 4 der EU-Verordnung (EG) Nr. 1107/2009 im Rahmen der Zulassung von Pflanzenschutzmitteln (PSM) in Deutschland und der Genehmigung von PSM-Wirkstoffen in der EU zuständig. Die Grundwasser-Expositionsbewertung wurde in Europa 2014 auf der Grundlage des mehrstufigen FOCUS-Ansatzes harmonisiert. Dies gilt insbesondere für die Bewertungsstufen 1 und 2, in denen die harmonisierten FOCUS-Modelle PELMO, PEARL und MACRO verwendet werden, um das Versickerungsverhalten von Wirkstoffen und Metaboliten auf der Grundlage des chromatographischen Fließens (Matrixfluss) in der ungesättigten Bodenzone abzuschätzen.

In Deutschland wird seit 2012 vorrangig das eindimensionale Simulationsmodell FOCUS PELMO in Kombination mit dem FOCUS-Hamburg-Szenario verwendet, um das Versickerungspotenzial von Wirkstoffen und ihren Metaboliten ins Grundwasser zu bewerten. Dieser Status quo in der nationalen Grundwasserrisikobewertung geht auf Expertenentscheidungen aus dem Jahr 1990 zurück und folgt der Annahme, dass ein sandiger Boden mit geringem Gehalt an organischem Kohlenstoff und ein atlantisch beeinflusstes Klima mit relativ hohen Winterniederschlägen eine ausreichend konservative (realistische Worstcase-) Boden-Klima-Kombination repräsentiert, um das Versickerungsverhalten von PSM-Wirkstoffen und deren Abbauprodukten unter landwirtschaftlichen Bedingungen in Deutschland abzuschätzen.

Es wird derzeit unter Wissenschaftlern und Regulatoren in Europa diskutiert, die standardmäßig verwendeten Szenarien-basierten FOCUS-Grundwassermodelle auf räumliche Versickerungsmodelle zu erweitern und diese zukünftig für regulatorische Entscheidungen zu verwenden. Mit dieser neue Modellgeneration sollen als Verfeinerungsoption neue Szenarien definiert und vulnerable Standorte für gezielte Grundwassermonitoringstudien identifiziert werden. Diese geplanten Anpassungen und Entwicklungen lassen die Frage aufkommen, inwieweit zusätzliche Wasserverlagerungsprozesse in der ungesättigten Bodenzone, wie z. B. präferentielles Fließen, Oberflächenabfluss, Zwischenabfluss und Drainage sowie Sorption in tieferen Bodenschichten in bestehende FOCUS-Modelle integriert werden sollten, um eine zuverlässige Vorhersage des Versickerungspotentials von PSM zu gewährleisten. So hatte beispielsweise die EFSA bereits kritisiert, dass landwirtschaftlich genutzte Flächen mit Böden, die zu Makroporenbildung neigen, von den bestehenden FOCUS-Modellen und Szenarien wahrscheinlich nicht abgedeckt werden.

Ziel des Projekts war es, zu ermitteln, welche Anpassungen in künftigen nationalen Grundwasserrisikobewertungen für PSM erforderlich sind, um eine angemessene und zuverlässige Vorhersage des Versickerungspotenzials von Wirkstoffen und ihren Metaboliten mit der Methode räumlicher Modellierung zu gewährleisten. Die Kalibrierung und Implementierung zusätzlicher Prozesse für den Wasserhaushalt und den Transport von PSM in der ungesättigten Bodenzone in PELMO, z. B. präferentielles Fließen, Oberflächenabfluss, Zwischenabfluss und Drainage sowie Sorption im Untergrund werden im Bericht diskutiert. Die Verfügbarkeit und Qualität nationaler Geodaten wurde evaluiert hinsichtlich einer Extrapolation der Modellierungsroutinen für diese Prozesse auf die unterschiedlichen Boden- und Klimabedingungen in Deutschland. Es wurde untersucht, inwieweit die Grundwasserbewertung beeinflusst wird, wenn andere Prozesse wie Oberflächenabfluss, präferenzielles Fließen und Drainage neben Matrixfluss berücksichtigt werden. Neue Szenarien wurden ausgewählt und analysiert, um Empfehlungen für mögliche Anpassungen des nationalen Grundwassermodellierungsansatzes zu geben.

Wissensstand zu Oberflächenabfluss, Makroporenfluss, Zwischenabfluss und Drainage

Es wurde eine Literaturrecherche durchgeführt, um die Frage zu beantworten, inwieweit Bodenwasserprozesse wie Oberflächenabfluss, präferenzielles Fließen, Zwischenabfluss und Drainage, die derzeit in nationaler Modellierung der Versickerung von PSM in das Grundwasser nicht berücksichtigt werden, für die Wasser- und Stofftransportbilanz in der ungesättigten Zone unter den in Deutschland herrschenden Boden- und Klimabedingungen relevant sind.

Seit 2000 ist der Oberflächenabfluss technisch als optionale Modellierungsroutine für die Bodenwasserbilanz in den FOCUS-Versickerungsmodellen PELMO und PRZM implementiert. Oberflächenabfluss wurde bereits in einem früheren Forschungsprojekt zur Entwicklung eines bundesweiten Grundwassermodellierungsinstruments für Deutschland berücksichtigt. Zur Implementierung einer Modellierungsroutine wurde der Curve-Number-Ansatz auf Basis der FOOTPRINT-Bodenklassifizierung verwendet, der ursprünglich für das Runoff-Modell GERDA (GEobased Run-off, erosion and Drainage risk Assessment for Germany) entwickelt wurde. Die Verwendung einer deutschen Bodenkarte mit größerem Maßstab erforderte im aktuellen Projekt eine Weiterentwicklung des verfügbaren Ansatzes.

Präferenzielles Fließen oder Makroporenfluss im Boden und in der ungesättigten Zone ist ein Prozess, dessen Bedeutung seit vielen Jahren Gegenstand intensiver wissenschaftlicher Forschung auf nationaler und internationaler Ebene ist. Schrumpfrisse in bindigen Böden, Bioporen durch Regenwürmer, aber auch strukturelle Unterschiede in der ungesättigten Zone in Bezug auf die Lithologie oder vertikal ausgerichtete Inhomogenitäten des Untergrunds sowie geologische Störungen in Ablagerungen wie Geschiebelehmen, Kalksteinen und anderen Festgesteinen werden als Faktoren für hydraulisch aktive Diskontinuitäten genannt, die den Wasserhaushalt und das Fließen und den Transport von Chemikalien im Untergrund beeinflussen. Gezielte langfristige Grundwassermonitoringdaten aus dem dänischen Programm zur Bewertung der Versickerung von Pestiziden (PLAP) geben Hinweise darauf, dass das Versickerungsverhalten von PSM durch präferenzielle Fließwege in Abhängigkeit von der Bodenart, dem Wasserhaushalt des jeweiligen Feldes einschließlich des Klimas sowie dem Zeitpunkt und der Dosierung der Ausbringung beeinflusst wird. Insbesondere in tonigen und schluffigen Böden können präferenzielle Fließwege in größerem Maße zur Versickerung von PSM beitragen. Aufgrund der Beschaffenheit der Böden in Deutschland ist davon auszugehen, dass ein erheblicher Teil der landwirtschaftlich genutzten Böden potenziell von präferenziellen Fließmustern betroffen ist. Diskussionen mit den Experten des Projektbeirats ergaben, dass es schwierig ist, alle Ursachen für präferenzielles Fließen und ihre räumlichen und zeitlichen Merkmale in einer wissenschaftlich fundierten Klassifizierung zu berücksichtigen, da wissenschaftliche Erkenntnisse und bundesweite Informationen und Geodaten manchmal nicht verfügbar sind. Es bestand jedoch auch Einigkeit darüber, dass ein Mangel an wissenschaftlichen Informationen oder Geodaten nicht dazu führen sollte, Makroporenfluss bei der Entwicklung räumlicher Modelle außer Acht zu lassen, da dies in bestimmten Gebieten unter bestimmten Wetterbedingungen sogar zu einer höheren Unterschätzung der Pestizidauswaschung führen könnte. Die Experten empfahlen die Entwicklung einer einfachen Bodenklassifizierung für die Umsetzung einer neuen Modellroutine für Makroporenfluss sowie die Kalibrierung auf der Grundlage verfügbarer Lysimeterdaten und Monitoringdaten aus dem dänischen PLAP-System vorzunehmen.

Es gibt verschiedene hydrologische Konzepte zum Zwischenabfluss oder hypodermischen Abfluss. Allgemein versteht man darunter einen schnellen Zufluss von versickertem Niederschlagswasser zu Oberflächengewässern in deutlich kürzerer Zeit als über den Basisabfluss. Im Rahmen des Projekts haben Experten diskutiert, dass ein schneller Zwischenabfluss über temporär hoch anstehendes Grundwasser ein Phänomen ist, das räumlich und zeitlich eher begrenzt auftritt. Zwischenabfluss unter der Oberfläche als schneller seitlicher

Transport im Untergrund oberhalb des Grundwasserkörpers tritt so gut wie nie auf, außer in Gebieten mit steilen Hängen in Kombination mit der Nähe zu Oberflächengewässern. Die Entstehung dieser lateralen natürlichen Abflüsse in der Uferzone ist zeitlich auf wassergesättigte Unterböden beschränkt. Aufgrund der geringen räumlichen Relevanz des Zwischenabflusses im Verhältnis zur landwirtschaftlichen Fläche in Deutschland und der Schwierigkeit, ihn in einem eindimensionalen Grundwassermodell zu implementieren, wurde beschlossen, den Zwischenabfluss nicht als Prozess für die Modellierung der Versickerungsneigung von PSM auf nationaler Ebene zu berücksichtigen.

Drainage als schneller unterirdischer Abfluss über künstliche Entwässerungsrohre in Oberflächengewässer kann nach Niederschlagsereignissen oder in Zeiten steigender Grundwasserstände auftreten. Künstliche Drainageanlagen sind in Deutschland teilweise weit verbreitet, insbesondere in den nördlichen Tieflandgebieten. Die derzeit für einige Bundesländer verfügbaren Karten von Drainagesystemen basieren größtenteils nur auf potenziell vorhandene Anlagen. Jeder in PELMO technisch umsetzbare Drainageansatz kann nur auf Basis von Sickerwasserraten entwickelt werden, da derzeit keine verlässlichen Informationen über Grundwasserspiegel und ihre saisonalen Schwankungen in drainierten Gebieten vorliegen.

Da Sorption an organischem Kohlenstoff im Boden einer der sensitivsten Parameter für die Vorhersage der Versickerung von PSM ist, ist eine Evaluierung tatsächlich gemessener Kohlenstoffgehalte in landwirtschaftlichen Böden in Deutschland, insbesondere im Unterboden, erforderlich und wurde daher in die Untersuchungen einbezogen.

Implementierung neuer Prozesse und Boden-Klima-Szenarien in GeoPELMO DE

Im Laufe des Projekts wurde beschlossen, eine neue Version von GeoPELMO DE für die landwirtschaftliche Fläche in Deutschland unter Berücksichtigung aktueller Geodaten zu entwickeln. Zur Parametrisierung des Wasserhaushalts und des Pestizidtransports in der ungesättigten Zone bis zu einer Bodentiefe von 1 m wurden bundesweit verfügbare Bodendaten im Maßstab 1:250.000 verwendet und bei Bedarf angepasst. Die GeoPELMO DE-Version aus einem früheren Projekt basierte noch auf Bodendaten mit einem Maßstab von 1:1.000.000, daher wurde ein Vergleich beider Bodenkarten in Bezug auf die tiefenabhängigen Gehalte an organischem Kohlenstoff durchgeführt. Eine statistische Analyse bundesweit verfügbarer gemessener Gehalte an organischem Kohlenstoff lieferte den Nachweis, die Humusklasse ‘0‘ durch Defaultwerte von 0,2 % in 0 bis 60 cm bzw. 0,1 % in 60 bis 100 cm Bodentiefe zu ersetzen, wobei beide Werte dem 30. Perzentil gemessener Werte für die Humusklasse ‘0‘ entsprechen.

Für die Implementierung von Klimadaten wurden Informationen von 299 Wetterstationen des Deutschen Wetterdienstes (DWD) berücksichtigt. Voraussetzung war, dass eine Wetterstation über tägliche Daten zu Lufttemperatur, relativer Luftfeuchtigkeit und Niederschlag sowie teilweise zur Evapotranspiration für den Zeitraum 1985–2010 verfügte. Die räumliche Zuordnung der ausgewählten Wetterstationsdaten zum deutschen Agrarraum basiert auf einer statistischen Analyse mit Rasterdatensätzen des DWD mit monatlichen Durchschnittswerten für Temperatur und Niederschlag für den Klimaperiode 1980–2009 und einer räumlichen Auflösung von 1 x 1 km. Es wurde ein Rasterdatensatz mit täglichen Wetterdaten mit einer Auflösung von 200 x 200 m entwickelt, um der Auflösung der Bodenkarte zu entsprechen.

Um die Modellierungsroutine für den Oberflächenabfluss in PELMO anzupassen, wurde der Curve-Number-Ansatz auf Basis der FOOTPRINT-Bodenklassifizierung auf alle Bodenprofile der deutschen Bodenkarte im Maßstab 1:250.000 angewendet, indem ihnen eine entsprechende PRZM-Hydrologische Bodengruppe (SHG) zugewiesen wurde. Die angewandte Methodik basiert auf einem Entscheidungsbaum mit mehreren Fragen, die für jedes Bodenprofil beantwortet werden mussten. Als Ergebnis dieser Klassifizierung werden 37,8 % der deutschen Ackerfläche als Boden der SHG A klassifiziert, die eher durchlässige Böden auf sandigen und kiesigen Substraten darstellen und häufig in Norddeutschland zu finden sind. Darüber hinaus werden 23,7 % der Agrarflächen als SHG B, 27,5 % als SHG B-C und 11,0 % als SHG C klassifiziert, die durch unterschiedliche Bodentexturen gekennzeichnet sind und bei denen die Neigung zum Oberflächenabfluss bei Starkniederschlagsereignissen mehr oder weniger zunimmt.

Es wurde eine Makroporen-Klassifizierung der Böden entwickelt, welche die Textur und einen sehr hohen Humusgehalt der Böden sowie das lokale Vorkommen von sehr oberflächennahen Grundwasserspiegeln berücksichtigt. Die Klassifizierung gibt hauptsächlich die Anfälligkeit der Böden für die Bildung und den Erhalt von Trockenrissen unter trockenen Wetterbedingungen wieder. Die Tendenz der Böden, Bioporen über einen längeren Zeitraum zu konservieren, wird durch diese Klassifizierung teilweise abgedeckt. Es wurde beschlossen, drei Vulnerabilitätsklassen zu entwickeln und die Makroporenklassifizierung auf eine Bodenprofiltiefe von 1 m anzuwenden. Etwa 12,3 % der deutschen Landwirtschaftsfläche werden mit einer Tendenz für hohen Makroporenfluss eingestuft, 52,9 % als potenziell anfällig für einen mäßigen Makroporenfluss und 34,8 % als nicht anfällig für Makroporenfluss. Letztere sind hochdurchlässige Sandböden, die vor allem in Norddeutschland vorkommen. In PELMO wurden ein statischer und ein dynamischer Modellierungsansatz entwickelt, um Makroporenfluss begleitend zum Matrixfluss zu parametrisieren. Sowohl der statische als auch der dynamische Ansatz wurden im Vergleich zur Standard-FOCUS-Modellierungsroutine in PELMO sowie unter Berücksichtigung einer erhöhten Dispersionslänge getestet. Um eine geeignete Tiefe des Makroporeneinflusses und den prozentualen Anteil des Makroporenflusses zu kalibrieren, wurden für mehrere Wirkstoffe und deren Metaboliten aus Langzeit-Drainagedaten der PLAP-Standorte Estrup und Silstrup für eine standortspezifische Modellanalyse verwendet. Die Vergleichsanalyse hat gezeigt, dass während der PLAP- und Lysimeter-Versuche auf nicht sandigen Böden präferentielles Fließen auftrat. Es wurde ferner beobachtet, dass die beiden FOCUS-basierten Modellroutinen in PELMO, die auf Matrixfluss mit standardisierter und erhöhter Dispersionslänge basieren, in den meisten Fällen nicht in der Lage waren, die experimentellen Daten abzudecken, insbesondere hinsichtlich der Höhe und des zeitlichen Durchbruchs der gemessenen Substanzen. Die in den verschiedenen Experimenten nachgewiesene Versickerung ließ sich am besten durch eine unterschiedliche Parametrisierung der Anteile des statischen und des dynamischen Makroporenflusses abbilden. Es war jedoch schwierig, eine exakte prozentuale Parametrisierung des Makroporenflusses zu finden, die für alle untersuchten Monitoring- und Lysimeterergebnisse gilt. Schließlich wurden die PLAP-Monitoringergebnisse für Axostrystrobin und seinen Metaboliten CyPM sowie die Lysimeterergebnisse für Isoproturon und Terbuthylazin verwendet, um eine niedrige bis mittlere Parametrisierung des statischen und dynamischen Makroporenflusses in GeoPELMO DE zu definieren. Unter Berücksichtigung der Bodenklassifizierung werden 12,3 % der landwirtschaftlichen Böden, die mit einer Tendenz zu hohem Makroporenfluss ausgewiesen sind, mit einem minimalen statischen Makroporenfluss von 4 % und einem dynamischen Makroporenflusses bis maximal 8 % in Abhängigkeit von den standortspezifischen Wetterbedingungen parametrisiert. 52,9 % der landwirtschaftlichen Böden mit einer Tendenz zu mäßigem Makroporenfluss werden mit 2 % statischem Makroporenfluss und einem dynamischen Makroporenfluss bis maximal 4 % parametrisiert. Für die restlichen 34,8 % der landwirtschaftlichen Fläche in Deutschland wird kein Makroporenfluss berücksichtigt. Der Auslöser für die Berechnung des Makroporenflusses mit dem statischen Mindestprozentsatz in PELMO ist eine tägliche Niederschlagsmenge von 10 mm. Abhängig von der Bodenfeuchte in den vorangegangenen 7 Tagen kann der dynamische Anteil des Makroporenflusses höher sein als der statische Anteil.

Um die Entwässerung durch künstliche Drainagerohre in GeoPELMO DE abzubilden, wurde beschlossen, sich auf potenziell drainierte landwirtschaftliche Flächen in Norddeutschland zu konzentrieren, da die Entwässerung durch Drainagen in der norddeutschen Tiefebene voraussichtlich eine größere Rolle spielt und relevante Geodaten in den nördlichen Bundesländern in größerem Umfang verfügbar waren. Anhand der verfügbaren Informationen wurden potenziell drainierte landwirtschaftliche Flächen in sieben Bundesländern in Norddeutschland definiert. Eine deskriptive statistische Auswertung potenziell drainierter Landwirtschaftsflächen in Schleswig-Holstein, Mecklenburg-Vorpommern, Brandenburg, Sachsen-Anhalt, Sachsen, Niedersachsen und Nordrhein-Westfalen wurde in Bezug auf Bodentypenklassen aus der Bodenkarte 1:250.000 durchgeführt, um potenziell drainierte Bodentypen auch in Brandenburg zu definieren, wo entsprechende Daten nicht verfügbar waren. Ein einfacher Entwässerungseffizienzfaktor (f_{eff}) wurde entwickelt und evaluiert, um die Entwässerungsraten über Drainagerohre auf der Grundlage der Sickerwassermenge aus der ungesättigten Bodenzone mit dem eindimensionalen Modell PELMO berechnen zu können. Mittlere Drainageraten wurden für mehrere Bodentypenklassen aus der Bodenkarte 1:250.000 ermittelt. Entsprechende räumliche Daten wurden aus drei Bundesländern in Norddeutschland zur Verfügung gestellt: Mecklenburg-Vorpommern, Niedersachsen und Sachsen-Anhalt. Die für die Bodentypen abgeleiteten unterschiedlichen Drainageraten wurden in GeoPELMO DE als Entwässerungseffizienzfaktoren (f_{eff}) für alle drainierten Szenarien verwendet. Da keine räumlichen Informationen über die Tiefenlage künstlicher Drainagesysteme und schwankende Grundwasserspiegel in Norddeutschland verfügbar sind, wurde in PELMO eine Standardbodentiefe von 80 cm definiert, um den Verlust an Drainageflüssen anhand simulierter Sickerwassermengen zu berechnen. Dahinter steht die Annahme, dass Entwässerungsrohre immer in einer Bodentiefe oberhalb häufig auftretender Grundwasserspiegel verlegt werden, die an verschiedenen Standorten variieren können. Da im regulatorischen Kontext jedoch die berechnete Sickerwasserkonzentration in 1 m Bodentiefe als Näherungswert zur Abschätzung der Grundwasserverschmutzung herangezogen wird, musste im Modell ein Kompromiss gefunden werden, die Drainage in einer entsprechend geringeren Tiefe als 1 m abzubilden. Modellierungsergebnisse mit PELMO zeigen, dass saisonale Entwässerungseffekte zu beobachten sind, wobei im Herbst und Winter höhere Drainageflüsse modelliert werden als im Frühjahr und Sommer.

Bundesweite Modellierungsergebnisse

Die neue Version von GeoPELMO DE wurde für drei fiktive Wirkstoffe (P1-P3) und zwei fiktive Transformationsprodukte (M1, M2) mit unterschiedlichen Abbauraten und Sorptionswerten sowie Anwendungen bei Mais und Wintergetreide getestet. Es wurden vier aufeinanderfolgende Simulationsschritte durchgeführt, bei denen Matrixfluss (1), Matrixfluss + Oberflächenabfluss (2), Matrixfluss + Oberflächenabfluss + Makroporenfluss (3) und Matrixfluss + Oberflächenabfluss + Makroporenfluss + Drainage (4) berücksichtigt wurden. Diese hatten zum Ziel, den Einfluss jedes neuen Bodenwasserprozesses auf nationaler Ebene zu analysieren. Als fünfter Schritt wurden zwei verschiedene Defaultwerte an Gehalt an organischem Kohlenstoff für die Humusklasse ‘0’ in den Unterböden getestet.

Bundesweite Ergebnisse des simulierten Bodenwasserhaushalts wurden hinsichtlich des Einflusses einzelner Bodenwasserprozesse analysiert. So wurde beispielsweise beobachtet, dass nur der Oberflächenabfluss die Evapotranspiration geringfügig reduziert, während andere Prozesse wie präferenzieller Fluss und Drainage keinen Einfluss auf die Evapotranspiration haben, da ihr Einfluss auf den Bodenfeuchtegehalt der oberen Bodenschichten in PELMO sehr begrenzt ist. Die Runoffmengen werden um maximal 10 % reduziert, wenn der Makroporenfluss in der Simulation berücksichtigt wird. Der Effekt ist relativ gering und die bewerteten Kulturen haben keinen wesentlichen Einfluss auf die Verringerung des Oberflächenabflusses. Die simulierten Drainagewassermengen hängen hauptsächlich von der Jahreszeit ab, wobei sie im Herbst und Winter etwa dreimal so hoch sind wie im Frühjahr und Sommer. Der Einfluss einzelner Bodenwasserprozesse auf die Sickerwassermengen ist sehr unterschiedlich. Bei Berücksichtigung des Oberflächenabflusses werden geringere Sickerwassermengen simuliert, wobei der Einfluss des Prozesses auf die jährlichen Versickerungsmengen eher begrenzt ist. Zwischen den beiden Kulturen Mais und Wintergetreide wurden nur geringe Unterschiede beim Oberflächenabfluss beobachtet. Der Einfluss des Makroporenflusses auf die Gesamtmenge des Sickerwassers ist bei beiden Kulturen vernachlässigbar, es wurden Unterschiede von etwa 1 % der jährlichen Sickerwassermengen berechnet. Im Vergleich dazu hat der Drainagewasserfluss einen größeren Einfluss auf die jährliche Sickerwassermenge. Es werden geringere Sickerwassermengen simuliert, wenn die Drainage berücksichtigt wird. Dieser Einfluss variiert jedoch auf nationaler Maßstabsebene, da nur ein bestimmter Anteil der landwirtschaftlichen Fläche in GeoPELMO DE potenziell drainiert ist. Die mit GeoPELMO DE auf Basis des FOCUS-Modellierungsansatzes (nur Matrixfluss) berechneten Perkolatmengen liegen in derselben Größenordnung wie die im Hydrologischen Atlas für Deutschland angegebenen Sickerwassermengen. Die räumlichen Abweichungen zwischen den beiden unterschiedlichen Ansätzen sind gleichmäßig verteilt und liegen überwiegend in der Größenordnung von bis zu +/-50 mm pro Jahr, können aber in einzelnen Regionen auch höher sein. Die zusätzliche Berücksichtigung der drei Prozesse Oberflächenabfluss, Makroporenfluss und Drainage reduziert die berechneten Sickerwassermenge insgesamt deutlich, wobei der Einfluss des Makroporenflusses eher vernachlässigbar ist. Das schlägt sich auch in den Abweichungen von den Sickerwassermengen im Hydrologischen Atlas nieder.

Die Verteilung der mit GeoPELMO DE modellierten landesweiten Sickerwasserkonzentrationen für Wirkstoffe und Metaboliten hängt von mehreren Bedingungen ab: Der Berücksichtigung von Oberflächenabfluss, Makroporenfluss, Drainagefluss und deren Parametrisierung, Substanzeigenschaften wie Sorption und Abbau, PSM-Anwendungszeiten und Kulturen sowie der Wahl des räumlichen und zeitlichen Perzentils. Bei Wirkstoffen führte die Berücksichtigung von Runoff und Drainage hauptsächlich zu reduzierten Sickerwasserkonzentrationen in 1 m Bodentiefe. Die Berücksichtigung des Makroporenflusses führte im Allgemeinen zu höheren Konzentrationen, wobei der Einfluss des Makroporenflusses selbst höher war als bei verschiedenen Parametrisierungen des Makroporenflusses. Der relative Einfluss von Oberflächenabfluss und Makroporenfluss war bei der Frühjahrsanwendung in Mais normalerweise höher als bei der Herbstanwendung in Wintergetreide, wobei beide Prozesse die Sickerwasserkonzentrationen in entgegengesetzte Richtungen beeinflussen.

Der Einfluss von Drainage war im Allgemeinen eher begrenzt, es wurden geringfügige Unterschiede zwischen den beiden modellierten Kulturen und Ausbringungszeitpunkten beobachtet. Da es saisonale Effekte des Drainagewasserflusses gibt, könnte der Einfluss der Drainage auf die Verringerung der Sickerwasserkonzentrationen bei Anwendungen im Herbst und Winter etwas höher sein. Unter gemeinsamer Berücksichtigung von Runoff, Makroporenfluss und Drainage in der Modellierungsroutine wurden für Wirkstoffe in den meisten Fällen höhere räumliche Median- und 80. Perzentil-Sickerwasserkonzentrationen berechnet als mit dem Standard-FOCUS-Ansatz. Es gab jedoch auch eine Situation (P1 als mobile, schnell abbaubare Substanz in Wintergetreide), in der niedrigere Sickerwasserkonzentrationen berechnet wurden. Die auf der FOCUS-Modellierungsroutine (nur Matrixfluss) basierenden vorhergesagten Sickerwasserkonzentrationen sind vor allem im nördlichen Tiefland Deutschlands höher, wo Gletscherablagerungen und sandige Böden häufig vorkommen.

In weiten Teilen Mittel- und Süddeutschlands werden steigende Konzentrationen vorhergesagt, wenn Oberflächenabfluss, Makroporenfluss und Drainage zusätzlich in die Modellierung einbezogen werden. Infolge der zusätzlichen Berücksichtigung dieser drei Prozesse kann sich die mit GeoPELMO DE vorhergesagte relative räumliche Vulnerabilität von Wirkstoffen für große Gebiete ändern.

Es wurde beobachtet, dass der Einfluss zusätzlicher Prozesse auf die geschätzten Sickerwasserkonzentrationen bei Metaboliten im Vergleich zu Wirkstoffen deutlich geringer ist. Oberflächenabfluss, Makroporenfluss und Drainage können sowohl zu einer Verringerung als auch zu einer Erhöhung der Metabolitenkonzentrationen im Sickerwasser führen. Es scheint, dass steigende Konzentrationen aufgrund von Runoff festgestellt wurden, wenn der Wirkstoff im Herbst ausgebracht wurde (Wintergetreide), und sinkende Konzentrationen, wenn der Wirkstoff im Frühjahr ausgebracht wurde (Mais). In Bezug auf Makroporenfluss oder Drainage ist es eher schwierig, den Zusammenhang zwischen steigenden oder sinkenden Perkolatkonzentrationen als Funktion verschiedener Bedingungen zu beschreiben. Dies ist auch auf die sehr geringen relativen Veränderungen der Metabolitenkonzentrationen im Sickerwasser infolge der Berücksichtigung dieser beiden Prozesse zurückzuführen. Schließlich wurden für Metaboliten bei Anwendungen im Frühjahr und Sommer etwas niedrigere räumliche Median- und 80. Perzentil-Sickerwasserkonzentrationen berechnet, wenn Oberflächenabfluss, Makroporenfluss und Drainage gemeinsam in der FOCUS-Modellierungsroutine in PELMO berücksichtigt wurden. Im Gegensatz dazu wurden für die fiktiven Metaboliten bei Anwendungen im Herbst und Winter leicht höhere räumliche Median- und 80. Perzentil-Sickerwasserkonzentrationen geschätzt, wenn diese Prozesse zusammen modelliert wurden. Sowohl leicht steigende als auch leicht sinkende Trends für Metaboliten scheinen hauptsächlich durch Konzentrationsänderungen aufgrund von Runoff verursacht zu werden.

Die Ergebnisse der räumlichen Modellierung sind sensitiv gegenüber dem Gehalt an organischem Kohlenstoff im Boden. Das Ersetzen der Humusklasse ‘0’ durch leicht veränderte Defaultwerte für den Gehalt an organischem Kohlenstoff führte zu relativ hohen Änderungen in den Sickerwasserkonzentrationen für Wirkstoffe und Metaboliten, die weitgehend unabhängig von den Kulturen, den Anwendungszeitpunkten und den räumlichen Perzentilen auftraten. Der Effekt ist jedoch für Metaboliten deutlich geringer als für Wirkstoffe. Es wird daher empfohlen, den Gehalt an organischem Kohlenstoff im Unterboden so umfassend wie möglich auf der Grundlage von Messwerten zu parametrisieren.

Einordnung des Hamburg-Szenarios in den Kontext bundesweiter Ergebnisse

Es wurde eine Analyse durchgeführt, um das Schutzniveau des FOCUS-Hamburg-Szenarios, welches derzeit in der nationalen Grundwasserexpositionsbewertung für PSM verwendet wird, im Vergleich zu den kumulativen Modellierungsergebnissen von GeoPELMO DE für die gesamte landwirtschaftliche Fläche in Deutschland zu bestimmen. Es war erwartbar, dass die anhand des Hamburg-Szenarios vorhergesagte Sickerwasserkonzentration im Vergleich zu den bundesweit modellierten Ergebnissen jeweils ein relativ hohes Perzentil darstellt. Eine Abdeckung von etwa 80 % der räumlich verteilten Ergebnisse würde zum FOCUS-Konzept passen, wonach das Hamburg-Szenario realistische ´worstcase´-Klima-Boden-Bedingungen in Deutschland repräsentiert. Basierend auf Berechnungen für einige fiktive und mehr reale PSM-Anwendungen deckt das FOCUS-Szenario Hamburg in den meisten Fällen nicht 80 % der bundesweiten Sickerwasserkonzentrationen ab. Wurde das FOCUS-Versickerungskonzept des chromatographischen Fließens (Matrixfluss) in GeoPELMO DE (Modellversion FOCUS L) eingestellt, so lagen die Sickerwasserkonzentrationen ermittelt mit Hamburg für sechs fiktive Wirkstoffsituationen zwischen 52 % und 70 % (arithmetischer Mittelwert: 61 %) und für 11 reale Wirkstoffe zwischen 58 % und 80 % (arithmetisches Mittel: 69 %) sowie zwischen 38 % und 80 % für 34 reale Metaboliten (arithmetisches Mittel: 61 %). Das bedeutet, dass das Hamburg-Szenario bei einer hohen Anzahl von Stoffen im Vergleich zur Modellversion FOCUS L das 80. Perzentil nicht erreichte. Die Berücksichtigung von Oberflächenabfluss, Makroporenfluss und Drainage zusätzlich zu der FOCUS-Modellierungsroutine (Modelversion FOCUS L+R+M+D) führte zu einer niedrigeren Rangfolge des Hamburg-Szenarios für Wirkstoffe und Metaboliten und eher zu einem mittleren räumlichen Perzentil im Vergleich zu den bundesweiten Ergebnissen. Die Sickerwasserkonzentrationen aus dem FOCUS-Szenario Hamburg repräsentierten eine größere Bandbreite für sechs Dummy-Wirkstoffsituationen zwischen 25 % und 66 % (arithmetischer Mittelwert: 46 %), für 11 reale Wirkstoffe zwischen 20 % und 80 % (arithmetischer Mittelwert: 46 %) sowie für acht Dummy-Metaboliten-Situationen zwischen 53 % und 80 % (arithmetischer Mittelwert: 67 %) und für 34 reale Metaboliten zwischen 18 % und 79 % (arithmetischer Mittelwert: 50 %). Die Mittelwerte für reale Transformationsprodukte waren niedriger als für Dummy-Metaboliten, vermutlich weil auch sekundäre, tertiäre und quaternäre Metaboliten in den realen Abbauschemen berücksichtigt wurden. Abschließend lässt sich feststellen, dass die Ergebnisse der räumlich verteilten Versickerungsmodellierung mit GeoPELMO DE für einen relativ hohen Anteil der untersuchten Wirkstoffe und ihrer Metaboliten konservativer sind als der derzeitig verwendete nationale Ansatz zur Risikobewertung Grundwasser. Diese Erkenntnis ist unabhängig davon, ob der FOCUS-Versickerungsansatz mit chromatographischem Fluss oder ein erweiterter Ansatz mit zusätzlichen Prozessen wie Oberflächenabfluss, Makroporenfluss und Drainage berücksichtigt wird. Die Perzentil-Rangfolge des FOCUS-Hamburg-Szenarios fällt jedoch geringer aus, wenn der Modellierungsansatz um Oberflächenabfluss, Makroporenfluss und Drainage ergänzt wird. Es wurde eine weitere Analyse durchgeführt, um den Anteil einzelner Prozesse an diesen Ergebnissen zu untersuchen.

Empfehlungen für die nationale Grundwasserrisikobewertung

Aus den beiden Modellversionen FOCUS L und FOCUS L+R+M+D von GeoPELMO DE wurden alternative Szenarien ausgewählt, die das 80. räumliche Perzentil der nationalen Klima-Boden-Bedingungen besser repräsentieren als das FOCUS-Hamburg-Szenario. Es wurde das Prinzip gewählt, Klima-Boden-Kombinationen in GeoPELMO DE zu identifizieren auf der Grundlage der höchstmöglichen Anzahl von Überschneidungen zwischen dem 75. und 85. räumlichen Perzentil aus 14 Sickerwasserkonzentrationskarten (drei Dummy-Wirkstoffe und vier Metaboliten in zwei Kulturen). Diese Szenarien wurden auch für reale Wirkstoffe und Metaboliten getestet. Die beiden Klima-Boden-Kombinationen 6739/2804/Barsinghausen-Hohenbostel und 6126/2620/Hohwacht können als alternative Szenarien für den FOCUS-Versickerungsansatz (FOCUS L) empfohlen werden. Beide Szenarien erreichten das 80. ± 5. räumliche Perzentil für die meisten der Dummy-Wirkstoffe und Dummy-Abbauprodukte. In wenigen Fällen lagen die geschätzten Sickerwasserkonzentrationen über dem 85. oder unter dem 75. Perzentil. Beim Vergleich der beiden Szenarien mit bundesweiten Ergebnissen für Wirkstoffe aus realen PSM-Anwendungen lag die räumliche Abdeckung zwischen 63 % und 85 % für 6739/2804/Barsinghausen-Hohenbostel und zwischen 73 % und 88 % für 6126/2620/Hohwacht, weitgehend unabhängig von den Eigenschaften der Substanzen. Bei den realen Metaboliten ist die Situation etwas anders. Die für 6739/2804/Barsinghausen-Hohenbostel simulierten Metabolitenkonzentrationen lagen im Bereich zwischen 40 % und 93 % und für 6126/2620/Hohwacht zwischen 43 % und 93 %. Diese Ergebnisse zeigen, dass mit beiden Szenarien das Schutzniveau nicht für alle real getesteten Metabolitensituationen erreicht wurde. Die Berechnung der Sickerwasserkonzentrationen für Metaboliten ist jedoch generell mit höheren Unsicherheiten verbunden. Daher scheinen die Ergebnisse für beide Szenarien auch für Transformationsprodukte noch akzeptabel zu sein.

Die sechs Klima-Boden-Kombinationen 6135/2620/Hohwacht, 3162/798/Ulm, 7344/2352/Bad Harzburg, 9854/10464/Burgwald-Bottendorf, 935/379/Grambek und 1945/570/Schleswig wurden in verschiedenen Schritten aus der Modellversion FOCUS L-R+M+D unter Berücksichtigung von chromatographischen und präferenziellen Fließen, Oberflächenabfluss und Drainage ausgewählt. Inwieweit sie letztlich das 80. ± 5. räumliche Perzentil für alle Dummy-Wirkstoffe und Dummy-Abbauprodukte abdecken, hängt von der

Anzahl der Überschneidungen in dem Auswahlschritt ab. Beim Vergleich der sechs alternativen Szenarien mit den bundesweiten Ergebnissen für Wirkstoffe aus realen PSM-Anwendungen wurde festgestellt, dass die für 6135/2620/Hohwacht, 3162/798/Ulm und 7344/2352/Bad Harzburg simulierten Konzentrationen, die mit GeoPELMO DE ermittelten Konzentrationen des 80. räumlichen Perzentils angemessen repräsentieren. Im Gegensatz dazu waren die Ergebnisse für 9854/10464/Burgwald-Bottendorf, 935/379/Grambek und 1945/570/Schleswig für Wirkstoffe deutlich heterogener und weniger protektiv. Für reale Metaboliten hat sich die Situation insgesamt als heterogener erwiesen. Dennoch repräsentieren die Szenarien 3162/798/Ulm und 6135/2620/Hohwacht überwiegend ein annäherungsweise 80. räumliches Perzentil der bundesweiten Sickerwasserkonzentrationen für Metaboliten. Die Ergebnisse für 7344/2352/Bad Harzburg, 9854/10464/Burgwald-Bottendorf, 935/379/Grambek und 1945/570/Schleswig sind dagegen für mehrere reale Metaboliten-Situationen weniger protektiv. Von den vier Szenarien ließen sich vor allem aus den beiden Szenarien 69854/10464/Burgwald-Bottendorf und 1945/570/Schleswig keine ausgewogenen Sickerwasserkonzentrationen für alle getesteten realen Metaboliten ableiten, obwohl sie für die Dummy-Metaboliten eine bessere Situation darstellten. Aufgrund dieser Bewertung werden sowohl 6135/2620/Hohwacht als auch 3162/798/ Ulm und mit Einschränkungen 7344/2352/Bad Harzburg als die am besten geeigneten alternativen Szenarien empfohlen, die im Vergleich zu den Ergebnissen von GeoPELMO DE (FOCUS L+R+M+D) zu den stabilsten Modellierungsergebnissen für Wirkstoffe und Metaboliten führten. Allerdings muss einschränkend festgestellt werden, dass es keine Garantie dafür gibt, dass ein räumliches Schutzniveau von 80 % durch diese drei einzelnen Szenarien für alle im regulatorischen Rahmen vorkommenden Pestizidanwendungen abgedeckt ist.

Unabhängig vom gewählten Szenario wurde festgestellt, dass bei den Berechnungen mit einer Klima-Boden-Kombination für den Wirkstoff und die nachfolgenden Metaboliten innerhalb eines Abbauschemas wiederholt eine große Bandbreite an Perzentilen auftrat. Das bedeutet, dass ein einzelnes Szenario kaum verwendet werden kann, um eine realistische ´worst-case´-Situation für alle Substanzen eines bestimmten Abbauschemas zu garantieren. Das 80. räumliche Perzentil in einem Modell wie GeoPELMO DE würde für den Wirkstoff und die verschiedenen Metaboliten eines Abbauschemas immer durch andere individuelle Klima-Boden-Kombinationen repräsentiert werden. Dieses Ergebnis wurde unabhängig von der Modellversion FOCUS L oder FOCUS L+R+M+D beobachtet. Allerdings waren die Ergebnisse heterogener, wenn zusätzliche Prozesse wie Oberflächenabfluss, Makroporenfluss und Drainage in die Modellierungen zur Abschätzung der Sickerwasserkonzentrationen einbezogen wurden.

Aus modelltechnischer Sicht lässt sich schlussfolgern, dass nur ein räumliches Modell wie GeoPELMO DE in der Lage ist, ein exaktes zeitliches und räumliches 80. Perzentil für alle Wirkstoffe und Metaboliten zu berechnen unabhängig von ihren Eigenschaften, ihrer Position im Abbauschema und unabhängig vom Anwendungsmuster der PSM. Die Verwendung eines einzigen Szenarios kann als Annäherung dienen, würde jedoch in einem konkreten Fall immer zu Abweichungen von den Ergebnissen einer Geo-Version des Modells führen. Es bleibt daher schwierig, die Verwendung einzelner Szenarien für unterschiedliche Stoffeigenschaften, Kulturen oder PSM-Anwendungsmuster zu empfehlen. Darüber hinaus lieferte der Vergleich bundesweiter Ergebnisse mit GeoPELMO DE mit Ergebnissen des FOCUS-Hamburg-Szenarios Hinweise darauf, dass Unsicherheitsfaktoren für die Bewertung von Wirkstoffen und Metaboliten erforderlich wären, wenn Simulationen mit dem derzeit verwendeten Hamburg-Szenario durchgeführt werden. Solche regulatorischen Entscheidungen sollten auf umfassenden und umfangreichen Modellierungsergebnissen basieren.

1 Background

For the authorisation of plant protection products (PPPs) in Germany and for the approval of active substances in the EU the Federal Environment Agency (UBA) is responsible for ecotoxicological and groundwater risk assessment. The protection of groundwater as important environmental habitat and resource for the production of drinking water has a high priority. According to Article 4 of the EU Regulation (EC) No. 1107/2009 PPPs shall not have any harmful effects on groundwater. According to EU Regulation (EC) No 1107/2009 uniform principles and methods are applied for risk assessment of PPPs in Europe, but at the same time national specific conditions shall be considered in an appropriate way. Essential harmonisation for groundwater risk assessment was therefore implemented with the tiered FOCUS (FOrum for the Co-ordination of pesticide fate models and their USe) approach (FOCUS 2001a, European Commission 2014). This particular applies for groundwater assessment in tier 1 and tier 2, where the harmonized FOCUS models PELMO, PEARL and MACRO are used to estimate leachate concentrations of active substances and their metabolites in 1 m depth of the unsaturated soil zone. Nine FOCUS scenarios, which are implemented in all three models, represent different soil, climate and crop growing conditions across Europe. However, it is the responsibility of the European member states to evaluate and decide which FOCUS scenarios adequately represent their national environmental and agricultural conditions and whether they are protective enough for national regulatory decisions (EFSA 2013, FOCUS 2000, 2002, 2009/2014).

Since 2012 the one-dimensional simulation model FOCUS PELMO in combination with the FOCUS Hamburg scenario is used in Germany to evaluate the leaching potential of active substances and their metabolites for groundwater (Holdt et al. 2011). In case that adsorption and/or degradation of a substance depends on the pH value in soil, the FOCUS Kremsmünster scenario can be in addition relevant for national groundwater risk assessments. The selection of the FOCUS Hamburg scenario for national groundwater risk assessment in Germany assumes that a sandy soil with low organic carbon content and an Atlantic influenced climate with relatively high precipitation in the winter represents a conservative (realistic worst-case) soil-climate combination for the leaching behaviour of active substances and their metabolites in the agricultural area in Germany. This status quo in the national groundwater risk assessment leads back to first expert judgement decisions in relation to the development of the German lysimeter guideline (BBA 1990). The presumption behind is that the amount of percolate water in sandy soils and the chromatographic flow are always higher than in non-sandy soils which therefore can be considered as realistic worst-case condition for the leaching of chemical compounds in the unsaturated soil zone. The organic carbon content in soil is assumed as parameter which has the greatest effect on the adsorption and retention of the organic chemicals during leaching. Hence, the estimation of the leachate concentrations of PPPs in 1 m of soil depth strongly depends on the amount of organic carbon content in soil.

Results from a Europe-wide FOCUS analysis indicate, that primarily the FOCUS Hamburg scenario represents realistic worst-case soil and climate conditions from major arable lands in terms of chromatographic flow in soil in Europe (Vanclooster et al. 2003). In a previous research project (Klein et al. 2019a, 2019b) a GIS based analysis was conducted with PELMO using national geodata to investigate the spatial representativeness and the level of protection of the FOCUS Hamburg scenario with respect to German environmental soil and climate conditions. The FOCUS model approach in PELMO was adjusted to soil profiles of the German soil map BÜK1000N (BGR 2007) and 20-years climate data from 299 weather stations (Deutscher Wetterdienst, DWD). The spatial distribution of percolate concentrations in 1 m soil depth in Germany was calculated with a new GISPELMO model version for different substance properties, crops and application times, and a statistical percentile analysis was carried out. Based on the results it was concluded that the environmental conditions in Germany are not suitable covered by the FOCUS Hamburg scenario. The FOCUS Hamburg scenario is not representing the 80th spatial percentile for the agricultural area in Germany, if the 80th temporal percentile out of 20 weather years is considered for the estimation of leachate concentrations. A lower organic carbon content in numerous German soils was identified by the authors as main reason for the underestimation of nationwide leachate concentrations (Klein et al. 2015, 2019b). It became obvious from the investigations in Klein et al. (2019b) and according to Düwel et al. (2007) that considering existing nationwide soil profile data, it is difficult to parametrise the subsoils with reliable organic carbon contents, because measured data are rarely available.

The extrapolation of the scenario-based standard FOCUS groundwater models to spatial distributed leaching models and their use for regulatory decision-making is currently intensively discussed in the scientific und regulatory community in Europe (e.g., Gimsing et al. 2019, Tiktak et al. 2020). The FOCUS tiered approach already considers spatial differentiated modelling and new scenario definition as refinement option in tier 3 for more specific predictions of leachate concentrations (European Commission 2014). Furthermore, spatial distributed leaching modelling has been identified as possibility to identify vulnerable areas for leaching, e.g., for site selection for targeted monitoring studies (Gimsing et al. 2019) or to mitigate the leaching risk. However, the inclusion of additional modelling routines in the FOCUS models as runoff, preferential flow and transport, interflow and drainage are discussed as opportunity and/or prerequisite for such comprehensive model adjustments (Tiktak et al. 2020), because these processes can influence the water balance in the unsaturated soil zone, especially for non-sandy soils. EFSA (2013) already criticised those agricultural used areas with soils prone to macropores are probably not suitable covered by the existing FOCUS models and scenarios which are based on chromatographic flow only, except the FOCUS Châteaudun scenario in MACRO.

Runoff has been already considered as additional process in the development of PELMO for a nationwide modelling tool for Germany, whereby preferential flow and drainage have not been part of the latest investigations (Klein et al. 2015, 2019b). It is recognized from the scientific discussion that FOCUS groundwater model parametrisation with additional processes for the water balance in the unsaturated soil zone can be a challenge, especially regarding preferential flow (Berg et al. 2014). The main task in the project is to calibrate new modelling routines on experimental and monitoring results under different and real soil and climate conditions. Therefore, the consideration and calibration of runoff, chromatographic and preferential flow, interflow and drainage in groundwater modelling, the extrapolation of new modelling routines to different soil and climate conditions by using geodata, and finally their impacts for regulatory decision making in a large country like Germany needs further research.

2 Objective of the investigations

The aim of the investigations is to identify which adaptations are required for national groundwater risk assessments for PPPs in future to ensure a suitable and safe prediction of the leaching potential of active substances and their metabolites by modelling. Currently, the one-dimensional model PELMO which considers only chromatographic (matrix) flow in soil is used in combination with one FOCUS scenario for national risk assessments in tier 1 and tier 2. According to EU Regulation (EC) No 1107/2009 new adjustments and methods shall be developed in the project which are consistent to the harmonized European groundwater tiered approach (European Commission 2014) and which cover national environmental conditions in an appropriate way. Relevant processes for the water balance and pesticide transport in the unsaturated soil zone, e.g., preferential flow, runoff, interflow and drainage as well as adsorption in subsoils, and how they can be implemented in PELMO are discussed in the project report. The accessibility and quality of national geodata is evaluated with the aim to extrapolate the leaching modelling routines to the total agricultural area in Germany. Therefore, a regionalisation step is required to transfer the common and new soil water balance modelling routines in FOCUS PELMO to all existing soil types and climate conditions. Improved scientific knowledge since the development of the European FOCUS groundwater modelling approach will be considered. Spatial distributed groundwater modelling enables to investigate the protection level of the current FOCUS Hamburg scenario for Germany and to identify vulnerable soil-climate conditions and regions. Recommendations will be derived from the analysis for a future national groundwater modelling approach.

The investigations are related to the following scientific and regulatory questions:

- To which extent additional processes like preferential flow, runoff, interflow and drainage are relevant in the unsaturated soil zone for leaching under consideration of existing soil and climate conditions in Germany?
- Which geodata can be used to develop a nationwide regionalisation approach to refine the leaching modelling routines in PELMO considering chromatographic flow, preferential flow, runoff, interflow and drainage?
- Which level of protection in space and time can be estimated for the current standard national groundwater scenario FOCUS Hamburg which mainly represents chromatographic flow and pesticide transport in sandy soils? To which extent is the level of protection influenced when other processes like runoff, preferential flow, interflow and drainage are considered?
- Which recommendations can be derived for a regulatory suitable and safe prediction of the leaching potential of PPPs in Germany by considering the current level of harmonisation of the groundwater modelling approach in the EU? Which adjustments are required for a future national groundwater assessment strategy and what are the regulatory consequences?

3 State of knowledge

Literature research was conducted to answer the question to which extent the four processes runoff, preferential flow, interflow and drainage, which are currently not considered in national pesticide groundwater leaching by modelling, are relevant for the water and mass balance in the unsaturated zone under existing soil and climate conditions in Germany.

3.1 Chromatographic flow and soil organic carbon content

The leaching models which are currently used for the approval of active substances in the EU and for national authorisations of PPPs in Germany according to the Regulation (EC) 1107/2009 are based on developments of the FOCUS activity (FOCUS 2000, European Commission 2014). In both, the national and the European estimation of groundwater concentration for pesticides, chromatographic flow through the soil matrix plays an important role since a long time. For national registration the first version of the chromatographic flow model PELMO was already released in 1991. First European guidance for leaching of PPPs into groundwater was developed 1995 with a description of the relevant models and their strengths and weaknesses (FOCUS 1995). Several Member States had developed national soil-climate-scenarios for the registration of plant protection products (PPPs), but no standard scenarios were available at EU level.

At this time leaching assessments in Germany were often based on experimental field lysimeter results which represented chromatographic flow and pesticide transport in sandy soils with low organic carbon contents typically existing in soils in Northern Germany (BBA 1990). The assumption behind was that the amount of percolate water in sandy soils and the leaching of active substances and metabolites due to chromatographic flow represents a realistic worst-case and covers all national soil and climate conditions. The development of leaching models based on chromatographic flow considers degradation and sorption in soil as predominant processes influencing the leaching behaviour of active substances and their metabolites.

Because the sorption parameters used in the models are standardised to the organic carbon content in soil, the estimation of the leachate concentrations strongly depends on the organic carbon content in the scenario definition. In Germany the organic carbon contents in typical soil profiles from lysimeter cores have been measured and considered for national groundwater scenario definitions. In the EU locations with relatively high rainfall amounts and with low organic carbon contents in soil were selected as realistic worst-case situations by FOCUS (2000). These scenarios have been defined independently of simulation models, but they have also been implemented in the models PEARL, PELMO and PRZM, and MACRO in case of Châteaudun (only FOCUS scenario considering preferential flow). Later, the scenarios were partly updated by FOCUS in order to increase the harmonisation between models and to remove inconsistencies (European Commission 2014). Since 2011 national groundwater modelling in Germany is performed by using FOCUS PELMO and the European FOCUS Hamburg scenario (Holdt et al. 2011).

Results from a GIS based analysis for Germany conducted with GISPELMO (version 1.0) based on the BÜK1000N (BGR 2007) indicate that low organic carbon contents in numerous soils are one main reason for the underestimation of nationwide leachate concentrations with the FOCUS Hamburg scenario (Klein et al. 2015, 2019b). In GISPELMO (version 1.0) chromatographic flow is the dominant process. At the same time, it became obvious from the investigations in Klein et al. (2019b) and according to Düwel et al. (2007) that considering existing nationwide soil profile data, it is difficult to parametrise the subsoils with reliable organic carbon contents, because measured data are rarely nationwide available.

Comparable results are provided from investigations with national soil data in the Netherlands. The authors could show that parametrisation of the subsoil scenarios in GeoPEARL NL with more realistic organic matter contents has a large impact on the spatial distributed modelling results. The authors concluded that national modelling results based on measured organic matter contents in GeoPEARL NL are less conservative than using the standard European FOCUS Kremsmünster scenarios. Safety factors of 5 and 10 are recommended to use for regulatory decision-making in the Netherlands based on tier 1 modelling results with FOCUS PEARL and the respective scenario (Berg et al. 2017).

Finally, an evaluation of actual measured soil organic carbon contents, especially for subsoils, for agricultural soils in Germany is still required and therefore part of the investigations in the following.

3.2 Macropore flow/preferential flow

The FOCUS tiered approach according to European Commission (2014), which is currently used in Europe under the Regulation (EC) No. 1107/2009 to assess the leaching risk of pesticide and their metabolites to groundwater, has been criticized by EFSA (2013) to not account for preferential flow and transport. EFSA recommended that "the use of FOCUS scenarios for national registration purposes would require a thorough investigation of specific parameters (e.g., preferential flow, (…)) in order to assess whether the protection goals are met" (EFSA, 2013, p. 7). This critic belongs to the lower tier scenario-based modelling (except the Châteaudun FOCUS groundwater model scenarios, which is seldom applied), but also to complex higher tier assessments, e.g. the use of groundwater monitoring data (Gimsing et al. 2018) and spatial distributed modelling approaches (Tiktak et al. 2020). Quantifying the degree of preferential PPP-transport occurring through different soils as an outcome of variable changing climatic conditions is a challenge for groundwater modelling (Berg et al. 2014).

Preferential flow in soil and the unsaturated zone through different kinds of macropores is a process intensely academically examined for many years on national and international level. The proof of the existence and the importance of macropore or preferential flow has occurred not only numerously by direct measurements in the unsaturated zone, but also by the analysis of the corresponding response function of the short-term increase of the groundwater table after precipitation which is not only linked to matrix flow.

Macropore flow or preferential flow with a not steady matrix flow down can take place in unstressed aquifers in loose rock, in cohesive and non-cohesive sediments and in solid rock (Johnston 1987). According to the current state of knowledge preferential flow mainly occurs in cohesive soils, but not only. Here, particular shrinkage cracks appear in short or seasonal dry time, which accelerate the leaching of seepage water as well as therein dissolved substances (Wessolek 2004). Bio-pores caused by earthworm activities in contrast can appear also in rather sandy soils. Especially in areas with a small unsaturated zone with shallow groundwater tables, bio-pores with rather low depths are in comparison to abiotic caused shrinkage cracks considerably relevant for the leaching of pesticides into groundwater. Besides, differences in the structure of the unsaturated zone referred to lithology can be considerably relevant for the formation of preferential flow pathways: From dry tracer experiments and comparable methods (e.g. Electrical Resistivity Tomography measurements) it is known that the seepage water considerably moves down faster in coarser sediments. Horizontal barrier layers can hinder especially the depth related movement. Together with inclined surfaces and enough lateral expansion they can lead to the appearance of interflow in surface waters and cause the reduction of the base flow and the groundwater recharge, respectively. But also, rather vertically oriented inhomogeneities of the substrate in the unsaturated zone are important. Hydraulic active discontinuities influencing the water balance and substance flow and transport can also exist in fractured media like fractured glacier clayey tills, limestones and solid rocks (Haarder et al. 2021, Klint et al. 2004, Rosenbom et al. 2008).

The appearance of preferential flow pathways in the subsoil is of essential meaning for the duration of the leaching of chemical substances into groundwater. Based on matrix-linked flow this can enclose a very long period. Under consideration of mean boundary conditions of the relevant controlling parameters (groundwater formation rate and summarised field capacities in the unsaturated zone) the leaching rate can be assumed around one meter per year. Nevertheless, the variation of the leaching rate amounts at least for one magnitude (half a year up to five years) and is additionally clearly strengthened by macropores. The whole duration of the leaching of a substance transported with seepage water in areas with deeper water tables (10 meters and more) can take up to several decades. However, it can be also shortened by macropore flow up to few days, especially with very shallow groundwater tables in lowlands. In such landscape situations soils with a high organic content preferentially appear in valley meadows with peat substrates in the moors in which the macropore flow was documented currently, e.g. in a TERENO area in the Eifel (Pütz et al. 2016).

The modelling on meso-or macroscale level causes a different challenge than on field scale based on scale problems. The process of the groundwater recharge after precipitation is mentioned exemplarily: According to the Darcy law a slow and virtually stationary infiltration process is assumed. Nevertheless, in many catchment areas the infiltrating water after strong rainfall can reach the groundwater table via macropores and preferential flow pathways within hours. The groundwater recharge phase after a rain event extends over few days. Wittenberg (2011) compared in the North German lowland at sandy matrix seepage water way lines in lysimeters to groundwater levels in the subterranean catchment area and confirmed the fast infiltration of water into the unsaturated zone. As a result of a precipitation event leaching is typically not a slow process but takes place by preferential flow paths essentially within few days. The fast, event-related transient process of groundwater recharge is important for the analysis and modelling of water and material transport into groundwater, as well as for a realistic evaluation of temporal variabilities. Nevertheless, it has to be differentiated between the primarily quantitative, impulse-steered groundwater recharge and the actual qualitative material transport which can last for an obvious longer period due to retardation processes.

There is knowledge that in clayey and silty soils the water flow in macropores can contribute to leaching of PPPs to large extents (Flury 1996, Kördel et al. 2003, 2006, 2008). Long term targeted groundwater monitoring data from the Danish Pesticide Leaching Assessment Programme (PLAP) provides evidence, that leaching pattern of plant protection products are influenced by preferential flow depending on soil types, water balance of the field including climate and application time and dose. Higher proportions of several active substances and metabolites applied in early summer and autumn in shallow groundwater or drainage water have been observed on agricultural fields with loamy soils (Rosenbom et al. 2015). A Danish evaluation provides evidence, that the leaching risk as monitored in PLAP is not always captured by the European regulatory groundwater modelling approach (Pullan et al. 2016). Comparable geologic parent material from marine and glacial deposits and comparable soil units exists in Northern Germany. Numerous other studies indicate a considerable preferential solute transport through soils being the rule more than the exception (Beven and Germann 2013; Beven 2018; Nimmo 2021; Nimmo et al. 2021). Müller (2005) provided a literature discussion, GIS analysis and groundwater monitoring data evaluation related to the characteristic of agricultural soils in Germany and their proneness to preferential flow for PPP leaching. Based on the results of the analysis it must be assumed that non-sandy cohesive soils with the potential to form macropores appear on a considerable portion up to 64 % of the agricultural area.

The consideration of preferential flow in numerical models to simulate the substance transport from the soil surface down to the groundwater surface would basically lead to an obvious more realistic assessment of the potential contamination of groundwater. However, a correct calculation of the water flow via macropores and the correct calculation of the portion of pesticides, which are in the macropores soil unit and/or the matrix soil unit, is difficult, because it depends on many circumstances in reality. Nevertheless, the different pathway flows and its intensities are well examined phenomena on a local scale, thus their transformation with universally valid model algorithms for adequate consideration at landscape level is rather difficult and there are currently no rules documented in literature. It concerns a typical upscaling problem to transfer heterogeneous data measured in the environment to which further research is required.

Based on the current state of knowledge regarding macropores in soil and the resultant preferential flow the following points can be summarised:

- Preferential flow in soils and the unsaturated zone is proved at local scale by various field measurements and experiences.
- Macropores occur primarily in silty and clayey soils under temporary dry conditions, their increasing formation can be estimated under climate change conditions.
- However, tracer experiments show that vertical flow of leakage water is much more rapid in coarse than in fine gravel sediments.
- Bio-pores appear in silty and clayey soils but also in sandy soils. They are important in areas with high groundwater tables (low distance to groundwater table).
- Horizontal inhomogeneities with broad lateral shapes are leading to lateral fluxes in the unsaturated zone inside or below soils.
- Preferential flow contributes to an important reduction of travel times to groundwater: travel times of many years, which are normally estimated, can be reduced down to several days, weeks or months.
- Therefore, it can be assumed that a considerable high portion of agricultural soils in Germany have the potential to form macropores.
- It is recognised that the macropore flow (or preferential flow) is an important pathway for leaching concerning to the vertical transport of water and chemical substances in the unsaturated zone.
- Consideration of preferential flow is therefore important for future modelling of pesticide transport with the FOCUS modelling tools. There are currently no fixed algorithms implemented in the standard FOCUS models and scenarios (except for the Châteaudun scenario in MACRO) to consider the macropore flow phenomena for leaching assessments.

3.3 Runoff

Since FOCUS (2000) surface runoff as important process for the soil water balance is technically considered in the FOCUS leaching models PELMO and PRZM. Consideration of surface runoff leads to a reduction of the percolate amount and the substance concentrations in the percolate at 1 m soil depth in the FOCUS scenarios. However, the current guidance for groundwater modelling determines that the existing runoff modules in PELMO and PRZM should not be used for regulatory decision-making in order to achieve a suitable conservative estimation of leachate concentrations and to achieve a harmonisation with FOCUS PEARL (European Commission 2014). In view of the regulatory intention in European Commission (2014) it seems to be a comprehensible decision, because current groundwater modelling is based on a very limited number of nine soil-climate scenarios in Europe. However, for evaluating the protection level of the FOCUS Hamburg scenario for Germany with a nationwide geo-version of a leaching model, the effect of surface runoff on percolate concentrations could be evaluated because runoff is obviously relevant for major parts of the agricultural area. Runoff has been already considered as additional process in the development of PELMO for a nationwide distributed modelling tool for Germany (Klein et al. 2015, 2019b). To still increase scientific reliability, it was analysed how relevant surface runoff is for agricultural areas in Germany and how it impacts the calculation of German-wide percolate concentrations with a model like PELMO.

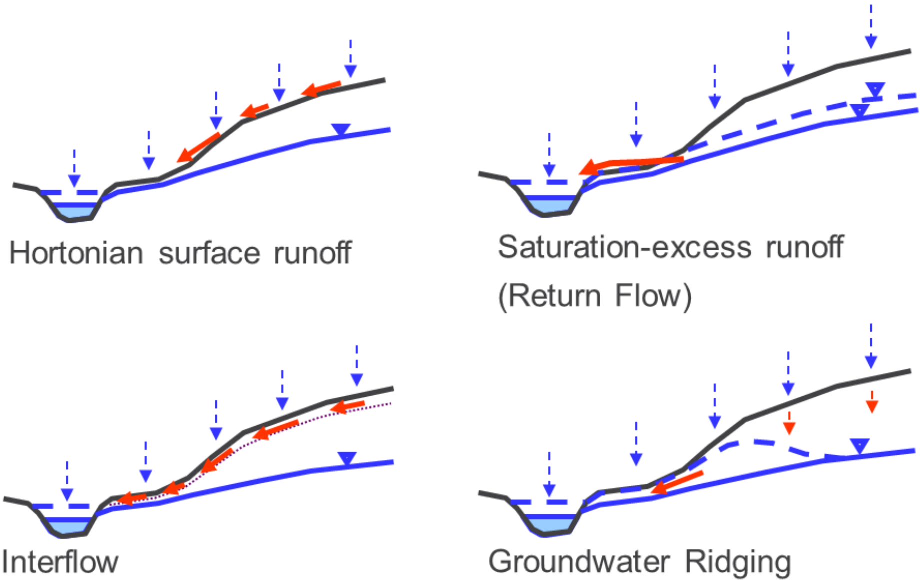
A broad overview about the hortonian surface runoff (see Figure 1) and how it is considered in current FOCUS models for surface water exposure assessments is provided in Bach et al. (2017). The curve number approach based on the FOOTPRINT soil type classification according to Dubus et al. (2009), which has been already used in several projects in Europe, was used to implement a modelling routine for runoff for a nationwide surface water model called GERDA (GEobased Run-off, erosion and Drainage risk Assessment for Germany). All soils from the German soil map BÜK1000N (BGR 2007) relevant for the agricultural areas were classified into 102 different FOOTPRINT soil types (FST). Each FST was assigned to a FOOTPRINT Hydrologic Group (FHG) which represents hydrological conditions for several processes influencing the soil water balance. All soils were finally classified into four different PRZM Soil Hydrologic Groups, which are characterised by different potential runoff amounts. The authors admit that the main uncertainty for nationwide modelling finally remains from the low number of soil reference profiles in the German soil map BÜK1000N (Bach et al. 2017, BGR 2007). The soil type classification according to Bach et al. (2017) was used for the surface runoff modelling routine for all climate-soil-scenarios in the first version of a nationwide groundwater model based on PELMO (Klein et al. 2019b). It has to be acknowledged that a German soil map BÜK250 with a larger scale has been recently published (BGR 2018b) und gives reason to further develop the curve-number approach for surface runoff used in both previous projects (Bach et al. 2017, Klein et al. 2019b).

3.4 Subterranean runoff/hypodermic flow

In the literature there are different hydrological concepts about interflow, for example hypodermic flow or direct flow or fast subterranean runoff, which all describe comparable phenomena. The process means a fast access of seeped precipitation water to surface waters (running waters or standing waters) in explicit shorter time periods than by the pathway base flow. The base flow is described as water flowing from the permanent saturated groundwater zone into surface waters independent from precipitation or snow melt events.

The effect of hypodermic flow as lateral process is currently not considered in the European and national risk assessments for groundwater by FOCUS modelling. The groundwater exposure assessment in FOCUS tier 1-3 is based on percolate concentrations at 1 m soil depth as a surrogate for groundwater concentrations (European Commission 2014). Hypodermic flow or subterranean runoff can occur above and below this depth in the unsaturated zone and temporary saturated zone, respectively. The generation of subterranean runoff (excluding hortonian surface runoff) can follow different processes and process understandings (Figure 1). Temporal saturation-excess (return flow), groundwater ridging and interflow can lead to subterranean runoff or hypodermic flow in the saturated zone (Lischeid 2017).

Figure 1 **Different processes generating surface runoff and subterranean runoff**



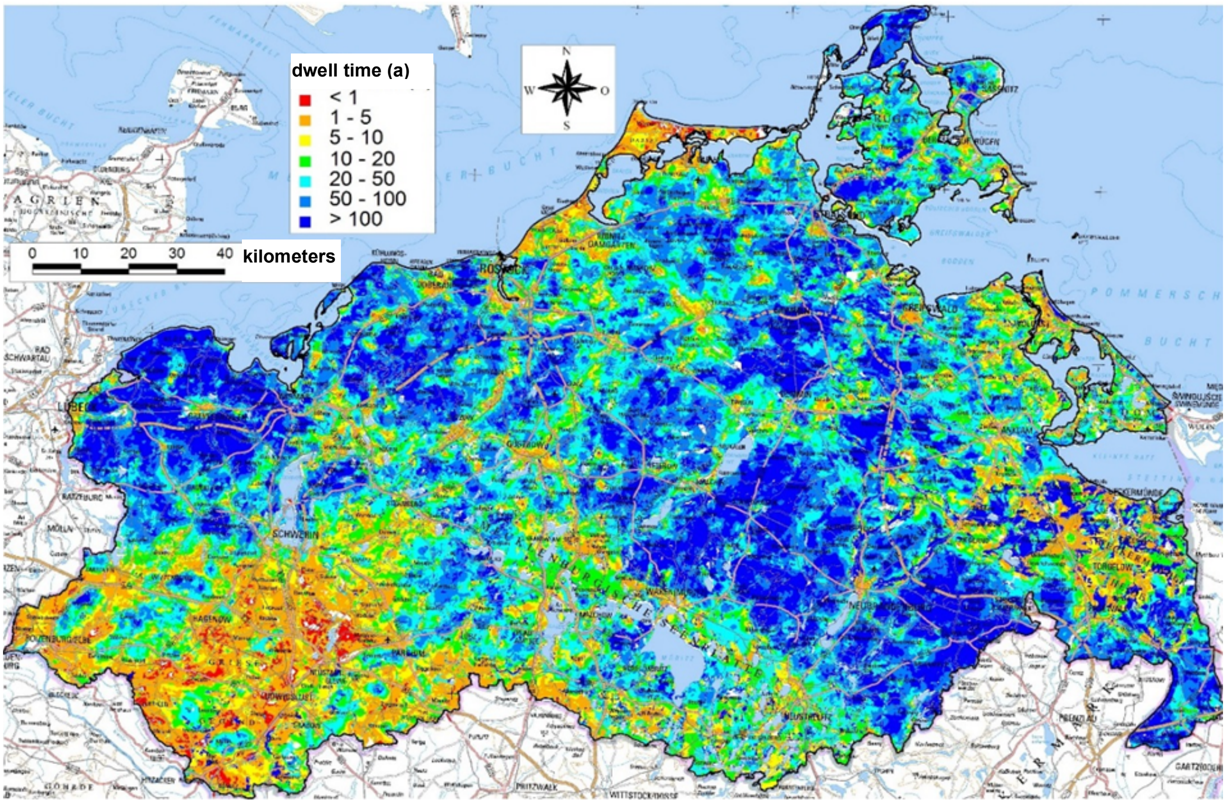
Source: Lischeid (2017)

It is a prevalent understanding that interflow appears in unconsolidated and solid rock areas equally whenever surface layers with distinct different hydraulic permeabilities appear within the unsaturated zone above the permanent groundwater table. In those conditions the seepage water or leachate is hindered in its vertical passage and flows along the inclined surface of the poorly permeable layer (e.g. $k_f < 1*10^{-5}$ m/s) down to the area section where it either can appear as a spring or drain directly into the next surface water. Interflow can locally be of great importance, because it can significantly shorten the transport of chemical compounds in hydraulically connected surface waters in comparison to the transport into deeper groundwater layers (Bronstert & Plate 1997).

Subterranean runoff (or hypodermic flow) and preferential flow can both lead to obvious quantitative changes of the infiltration of PPPs into groundwater aquifers. The extent of change depends on local and regional geological characteristics and hydrological situation in the unsaturated zone. It is common understanding of both processes that they appear predominantly in areas of cohesive, seepage water inhibiting rocks, sediments or soils, e.g. in the North German lowland and unconsolidated rock area with dominant agricultural land use. In comparison to the sandy soils on fluvioglacial sediments, areas in Northern Germany prone to both processes are mostly represented by fertile soils on loess, loam or marl deposits.

In the central parts of Mecklenburg-West Pomerania, for example, with a wide spreading of glacier till deposits and according to deep groundwater tables, calculated dwell times can vary from several decades up to 100 years or more (Figure 2). Here, the seepage water has to migrate through the very poorly water carrying, cohesive, clayey and silty substrates. Nevertheless, preferential flow is not considered in the calculation and can locally shorten the infiltration time into groundwater.

Figure 2: Dwell times of the seepage water in the groundwater cover in Mecklenburg-West Pomerania



Source: own illustration HYDOR according to Hannappel et al. (2011)

The standard calculation of the groundwater recharge usually considers the reduction of the subterranean or hypodermic run-off as well as surface runoff, e.g. according to DIN 4049, or in the Hydrologic Atlas of Germany (HAD) calculated by Neumann & Wycisk (2002). However, this standard method on regional or nationwide level does not fully considers local conditions and process understanding on a catchment scale.

Lischeid (2017) confirms that fast interflow via perched (intermitted) groundwater is rather a limited phenomenon. Subsurface interflow as rapid lateral transport in the subsurface above the groundwater body does hardly exist, except in areas with steep slopes in combination with vicinity to surface water bodies. The generation of those lateral natural drain flows in the riparian zone, especially stormflows, are temporally limited to water saturated subsurface soils (see interflow in Figure 1). This was confirmed by evaluations at catchment scale, which provide evidence for a hydrochemical stormflow response due to mobilisation of pre-event soil solution in the topsoil layer of the saturation zone. Other investigations show that even in catchments with proven long-distance lateral preferential flow and very steep slopes interflow comprises only a minor fraction of total stormflow (McGlynn & McDonnell 2003).

Regarding the project task to develop a nationwide modelling approach based on the agricultural area in Germany by considering the process understanding from Lischeid (2017), the area portion where interflow occurs in relevant amounts is rather small. In comparison, the national HAD approach to develop the groundwater recharge map was generated to quantify the available groundwater amounts rather than to quantify the depth and dynamics of interflow and is therefore, not recommended as useful approach for the project framework. Using the HAD approach to spatially calculate the groundwater recharge would massively overestimate the interflow component for agricultural areas. Due to the minor spatial relevance of the interflow related to the agricultural area in Germany and due to a difficult implementation in a one-dimensional groundwater model, it was decided not to consider interflow as relevant process for pesticide leaching or not to consider the areas where it occurs. As a consequence, seepage or percolate water is used in this project as reference for calculating pesticide leachate concentrations without subtracting interflow.

3.5 Drainage

Drainage as fast subterranean flow via artificial drainpipes into surface waters can also appear after precipitation events and lower the percolate amounts reaching groundwater. Percolate losses due to drainage systems are currently not considered in pesticide risk assessments for groundwater. This is different for the risk assessment for surface waters where surface runoff and drainage are recommended by FOCUS as relevant processes already since 2001 (FOCUS 2001b). However, the precondition for both modelling approaches is different. Because drainage and runoff are considered as main entry routes for surface waters, both processes need to be considered in the currently used and simplified scenario-based modelling approach. Because current FOCUS groundwater modelling to estimate percolate concentrations at 1 m soil depth is also based on a very limited number of simplified scenarios, a reduction of percolate amounts by drainage losses cannot easily be considered in lower tier groundwater assessments. However, for evaluating the protection level of the FOCUS Hamburg scenario for Germany with a nationwide geo-version of the model, the effect of artificial drainage systems on percolate concentrations could be evaluated because drainage systems exist in major parts of the agricultural area. To increase scientific reliability of this evaluation it is further analysed how relevant drainages systems are for agricultural areas in Germany and how they influence the calculation of percolate concentrations in a model like PELMO.

Especially in the North German lowland regions artificial drainage installations play an important role. Drained areas were identified in parts of the North German Lowlands (e.g. in Lower-Saxony and Mecklenburg-West Pomerania) by interpreting aerial photographs (Tetzlaff et al. 2008, 2009) and used as test regions to map potential drained areas to a wider extent. Typical site conditions of the identified drained fields were derived. A very high amount of groundwater recharge can locally contribute to drainage flows. In large regions in Mecklenburg-West Pomerania, for example, groundwater recharge takes in a portion of only about 50 % of total precipitation. The difference is mainly caused by drainage flow and surface runoff and natural interflow can be neglected here. As a consequence, water and pesticide losses through drainage systems are relevant to a high extent and cannot be fully ignored for spatial distributed leaching estimations in agricultural areas in Germany. However, the available maps from some federal states on drainage systems are to a wide extent based on potential drainage systems, only. There is some uncertainty here since there is no information about functionality and effectivity, respectively. Drainage systems are often located at locations with high groundwater levels. However, information about the installation depth of drainpipes is usually not available.

Long-term measurements of drainage amounts and pesticide rates in Denmark provide evidence that the occurrence of drainage in the fields is usually influenced by increasing water tables mostly in winter time. The seasonal amounts of drainage are influenced by shallow groundwater and different processes influence the pesticide concentration in the drained subsoils. However, tile drain flow (and fast lateral substance transport into surface water) can additionally be observed even if the temporal groundwater table is below the drains because macropore systems in the unsaturated soil zone are partly connected to the tiles. Dilution of pesticide concentrations in tile drainwater must be expected due to a higher amount of water transport in the tile drains if the groundwater table raises and the soil zone (with pesticide residues) is temporarily saturated (Brüsch et al. 2016, Rosenbom et al. 2015, 2021). However, any drainage approach possible to technically implement in PELMO could only consider percolate water since there are no reliable information currently available about groundwater tables and their seasonal fluctuations in drained areas. Comparable seasonal effects of drainwater fluxes have been observed at 11 sites in Germany and across Europe. A median water flow of 23 % of the yearly precipitation rates was measured in artificial drainage systems, varying from lower rates of 9 % in summer and higher rates of 54 % in winter (Hirt et al. 2011).

4 Implementation of new processes and nationwide scenarios in GeoPELMO DE

Chromatographic flow, macropore flow or preferential flow, surface runoff and artificial drainage have been discussed and identified as relevant processes to influence nationwide leaching modelling results for PPPs. It was decided to develop a new model version GeoPELMO DE which considers those processes for the whole agricultural area in Germany. Because chromatographic flow is already considered as standard modelling routine in PELMO, a soil and climate scenario definition based on geodata is required to nationwide adapt this process. Additional modelling routines and scenario parametrisations are required to implement macropore flow or preferential flow, surface runoff and artificial drainage in GeoPELMO DE. Chapter 4 provides geodata evaluations and methodic approaches for the implementation of new processes and nationwide soil -climate scenarios in GeoPELMO DE.

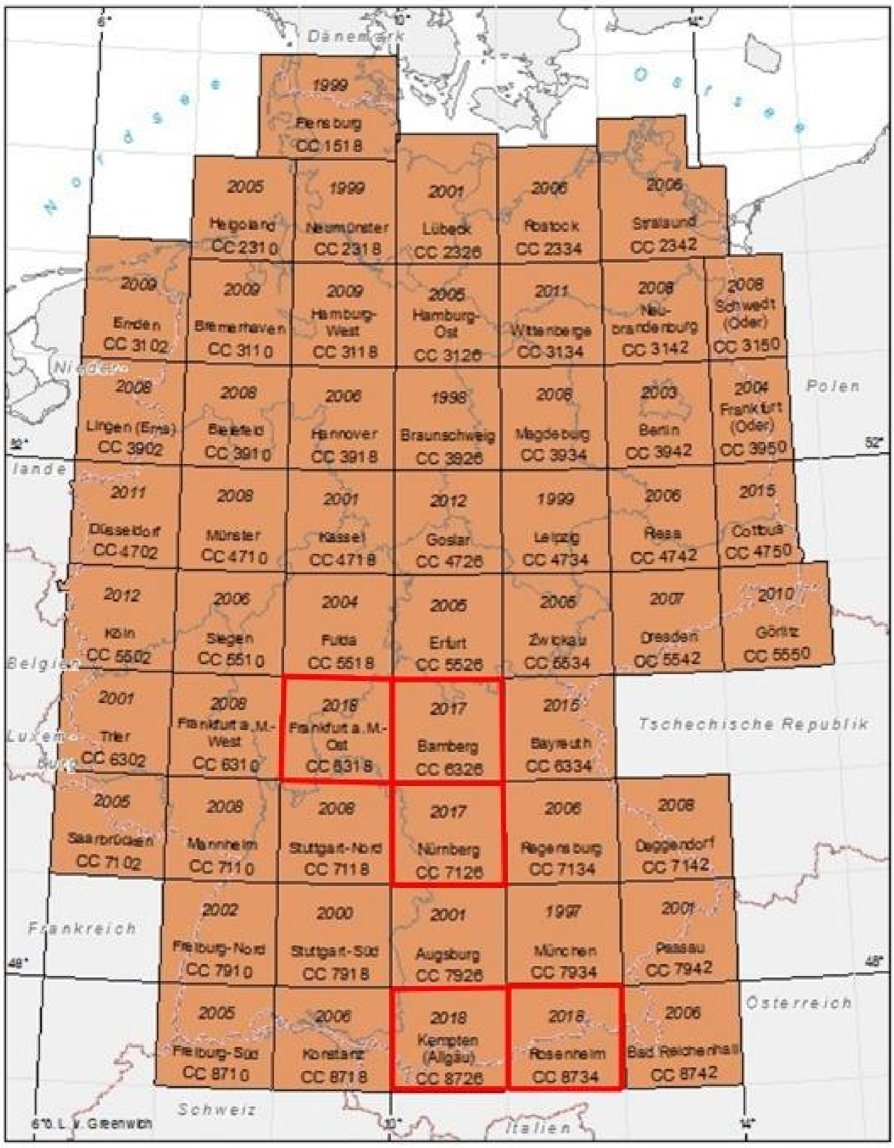
4.1 Soil Overview Map of Germany BÜK200 and BÜK250

The General Soil Map of Germany in the scale 1:200,000 (BÜK200) was developed by the BGR (Federal Institute for Geosciences and Natural Resources) in cooperation with Geological Services of the Federal States in Germany (BGR 2018a). The soil map was first published in the same sheet line system format like the TÜK200 (Topographical Map in the scale 1:200,000) and contains 55 single map sheets. The pedological data connected to the BÜK200 is stored in a relational database and used to demonstrate the abundance and the associations of soils and their basic properties in Germany. 50 map sheets have been available at the beginning of the project in 2017 (BGR 2017) and were used for evaluations of nationwide organic carbon soil contents (chapter 4.2.1.1 and 4.2.1.2). In 2018 the BGR published a new version of the General Soil Map with soil geometry data of the BÜK250 available for the whole area of Germany (BGR 2018b). The geometries of the BÜK200 (BGR 2018a) and the BÜK250 (BGR 2018b) are identical, and the soil attribute data can be joined via the same identification key (GEN_ID). This latest version of the BÜK250 was finally used for the implementation of nationwide soil scenarios in GeoPELMO DE.

The soil database is separated into geometry data in the form of a GIS compatible data format and the attribute data which are stored in different database tables. The attribute data can be joined to the geometry data by an identification key. The soil data base contains information about 8502 soil profiles. For 7540 soil profiles attributes for different soil horizons are provided. Figure 4 shows the number of available soil profiles with existing horizon data differentiated by land use type. All soil profiles with the land use types arable land and permanent crops were selected for further considerations in the project.

Figure 3: Map tiles of the BÜK200

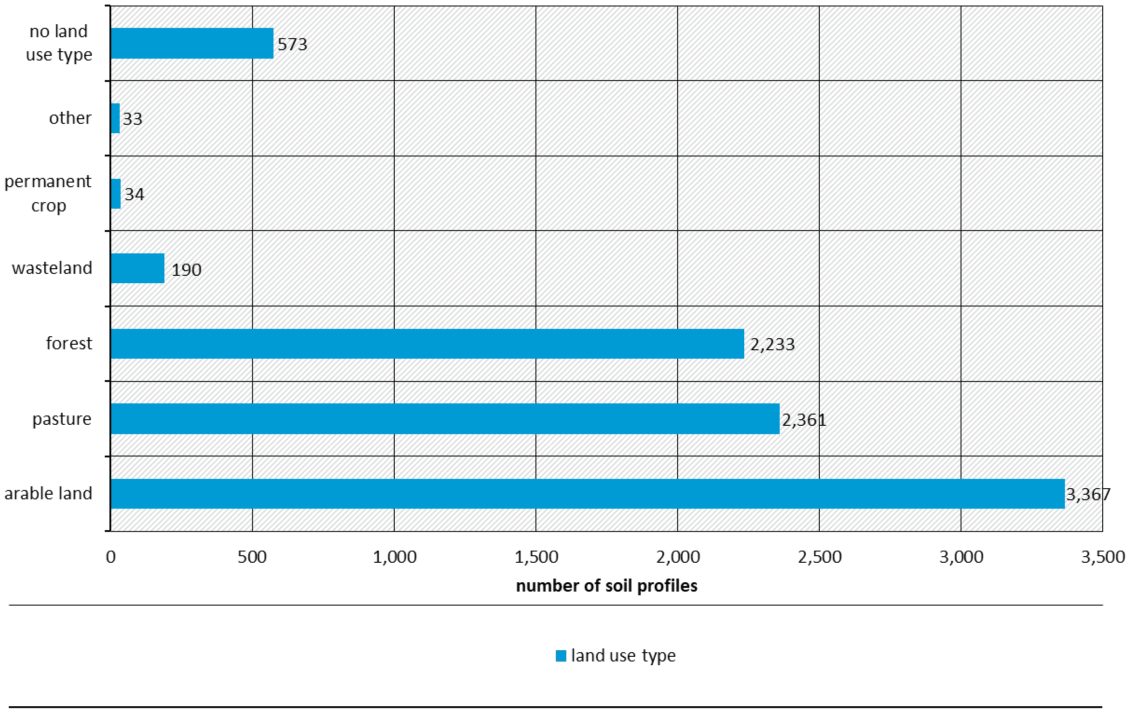
The five red outlined map tiles were not available 2017 at the beginning of the project.



Source: BGR (2018a).

Compared to the BÜK1000N (BGR 2007) the BÜK200 (BGR 2018a) is a distinctively improved soil database. About 3400 soil profiles for the land use types arable land and permanent crops are available (compared to only 129 in the BÜK1000N). Using the BÜK200 soil data base leads to a new challenge since there is often more than one soil profile defined for a single soil polygon based on the GEN_ID. The BÜK200 contains about 1300 GEN_IDs, for which one or more soil profiles with the land use type arable land and/or permanent crops are assigned. To limit the computational effort for the subsequent calculations with GeoPELMO DE it was decided to use only the dominant soil profile per GEN_ID (i.e. in total 1343 soil profiles with attribute data). The latest version of the BÜK200 soil attribute database (version 0.4), which was released in summer 2018, contains this necessary information and was used for soil scenario parametrisations in GeoPELMO DE (BGR 2018a).

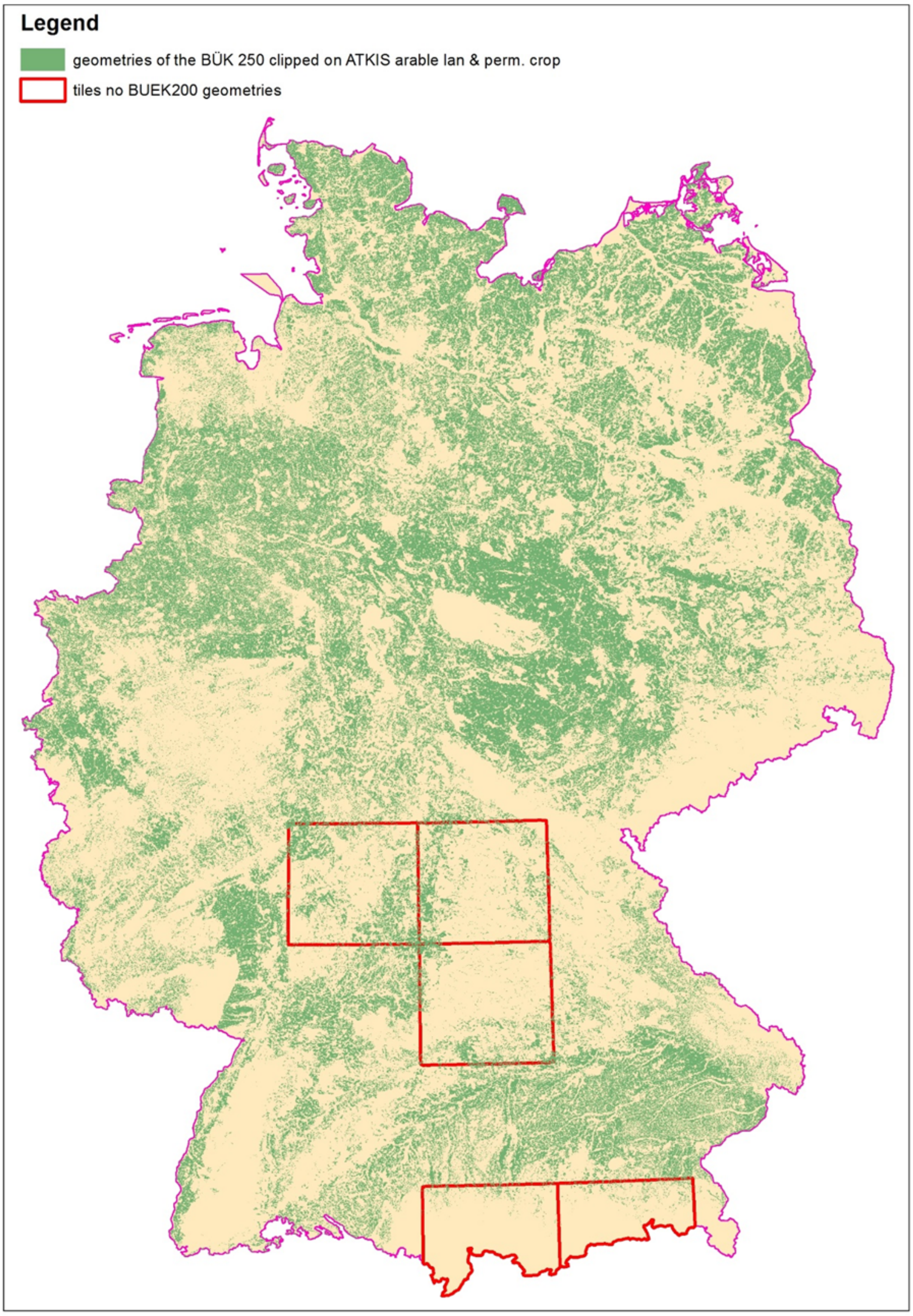
Figure 4: **Number of soil profiles of the BÜK200 (attribute database V 0.4, BGR 2018a) with horizon information differentiated by land use type**



Source: own illustration, RLP AgroScience

The soil map geometries in the soil data base can be connected to more than one land use type. For example, both land use types arable land and pasture can be defined with a specified area fraction. But in a GIS containing the BÜK250, only one land use type can be defined or illustrated for the whole polygon geometry. Consequently, areas with the land use types arable land and permanent crops can be overestimated. This is considered for further map analyses and soil implementation routines in GeoPELMO DE, when the exact location of soils defined with the land use types arable land or permanent crops was more important. The geometries of the BÜK250 (BGR 2018b), which contain both land use types arable land and permanent crops, were therefore additionally clipped by the ATKIS Basis DLM dataset to avoid an overestimation of the agricultural area in Germany (see Figure 5).

Figure 5: **Geometries of the BÜK200/BÜK250 clipped on ATKIS land use types arable land and permanent crops**



Source: own illustration, RLP AgroScience (according to BGR 2018a, 2018b)

4.2 Chromatographic flow

Chromatographic flow is the dominant process in the GISPELMO version 1.0, based on the standard modelling routine in FOCUS PELMO (Klein et al 2019b). The soil scenario parametrisation in this first GIS model version of PELMO for Germany was based on the soil data from the BÜK1000N (BGR 2007), Düwel et al. (2007) and Utermann et al. (2009). However, with regard to the soil information it is intended to improve the quality of the model by using the soil profile data and geometries from the BÜK200 and BÜK250 (BGR 2018a, 2018b).

The same climate data like in GISPELMO 1.0 are used in the GeoPELMO DE version 2.0 (Klein et al. 2019b).

4.2.1 Soil data and scenario parametrisation

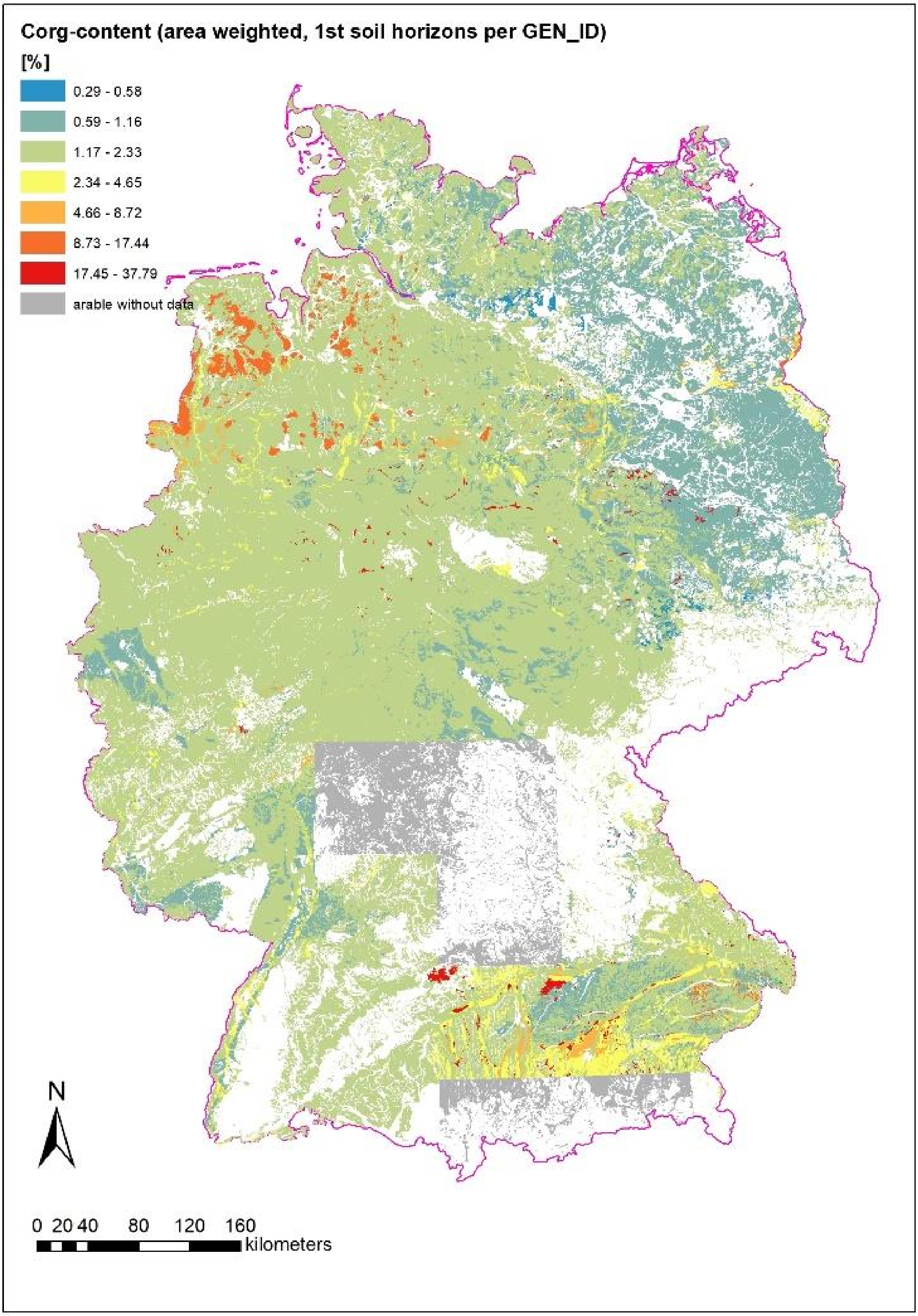
4.2.1.1 Comparison of nationwide soil organic carbon content with the FOCUS Hamburg scenario

It is known in general that the organic carbon content in soil is a sensitive parameter in the FOCUS groundwater models to estimate leaching concentrations of PPPs. Therefore, scenario definitions with realistic and suitable organic carbon contents in different soil depths is a crucial requirement for spatial distributed leaching modelling. Klein et al. (2019b) found out that based on the German Soil Map BÜK1000N (BGR 2007) the FOCUS Hamburg scenario is not suitable to cover all environmental conditions in Germany for PPP leaching and the 80th spatial and 80th temporal percentile was not achieved. A low organic carbon content in numerous German soils was identified as a possible reason for higher nationwide PPP leachate concentrations compared to the FOCUS Hamburg scenario. However, it was discussed that the soil profile data in the BÜK1000N (BGR 2007) are probably from limited coverage and accuracy for such an evaluation. A comparing analysis of soil organic carbon contents in Germany is therefore conducted with the new available soil data of the BÜK200 (BGR 2017) and the FOCUS Hamburg Scenario.

As a first analysis, an area weighted average calculation of the organic carbon content differentiated by depth classes is provided. As a second analysis, an area and depth weighted average calculation of the organic carbon content for all soils is provided. Soil data assigning to 50 out of 55 map sheets have been available at the time the comparing analysis was conducted (see Figure 6, BGR 2017). Only soil profile data representing agricultural soils were used for the analysis. The main procedure to prepare and analyse the soil data is provided in the following.

All soils with the land use type arable land or permanent crops were identified, which are most relevant for the use of PPPs. Because the humus content in the BÜK200 soil data base is provided by class values only, the class midpoint values according to the BKA 5 (2005) were used for subsequent calculations (Table 1). The humus contents in the table ‘Horizonte’ were converted to the organic carbon content values by dividing with the factor of 1.72. The organic carbon contents were assigned to the soil horizons. Figure 6 shows the distribution of the area weighted organic carbon contents of the 1st soil horizons from all soil profiles of the BÜK200 for arable lands and permanent crops.

Figure 6: Area weighted organic carbon content of the 1st soil horizons for arable lands and permanent crop (BÜK200)



Source: own illustration, RLP AgroScience (according to BGR 2017)

Table 1: Overview of the humus-classes and the organic carbon contents according to BKA 5 (2005)

Humus class (symbol)	Humus content mass [%]	Humus content class midpoint [%]	Organic carbon content (mass at class midpoint) [%]
h0	0	0	0
h1	< 1	0.5	0.29
h2	1 to < 2	1.5	0.87
h3	2 to < 4	3.0	1.74
h4	4 to < 8	6.0	3.49
h5	8 to < 15	11.5	6.69
h6	15 to < 30	22.5	13.08
h7	>= 30	65.0	37.79

To calculate the area weighted average analysis of soil organic carbon contents the area sizes of the map polygons from the BÜK200 had to be linked to the soil profile and horizon data in the soil data base. Therefore, the area sizes of the 'GEN_ID'-geometries identified in the GIS, where joined to the table with the soil profile data. Based on the information about the area fraction of the soil types (one single soil type is defined by a 'BF_ID') in relation to the total area of a 'GEN_ID'-geometry the area sizes of the 'BF_IDs' were calculated. Afterwards this value was allocated to every soil horizon of a 'BF_ID' in the table 'Horizonte'.

The calculation of the area weighted average of the organic carbon content in German soils was conducted separately for the soil depths 0 – 30 cm, 30 – 60 cm, 60 – 75 cm, 75 – 90 cm and 100 – 200 cm to be comparable to the FOCUS Hamburg soil scenario in PELMO. Since the horizon extents of most soil profiles of the BÜK200 do not match in most cases to the boundaries in the FOCUS Hamburg scenario, a simplified conversion approach was applied: First, the depth related midpoints of the soil horizons were identified by calculating the difference of the lower and upper boundary of each soil horizon. To determine the area related average of the organic carbon content for the depth 0 – 30 cm, all soil horizons of the BÜK200 soil profiles were selected whose depth related midpoint lies between 0 and 30 cm. The same procedure was used for all other analysed soil depths. In the next step the spatial relationship between the agricultural area and the organic carbon content of the soil horizons was generated. This was done by implementing an organic carbon-area-factor, which was calculated by multiplication of the organic carbon content with the area size of a soil horizon. Finally, all organic carbon-area-factors for each analysed depth were summarized and then divided by the total area of the included horizons. The results of the area weighted average organic carbon contents for all considered soil depths in comparison to the FOCUS Hamburg scenario is provided in Table 2.

Independent on whether organic surface layers are considered for the area weighted average calculation of the organic carbon content of agricultural soils in the depth 0 – 30 cm, both values (1.8 % and 1.7 %, respectively) lay distinctively above the organic carbon content of 1.5 % of the FOCUS Hamburg scenario in the same depth. In the deeper soil layer of 30 – 60 cm the average value of 0.5 % calculated based on the BÜK200 (BGR 2017) lies distinctively below the value in the FOCUS Hamburg scenario (1.0 %). In all subsoil layers below 60 cm soil depth (60 -75 cm, 75 – 90 cm, 90 – 100 cm and 100 - 200 cm) higher average organic carbon contents are observed compared to the FOCUS Hamburg scenario. Hence, in most of the analysed soil depths there are higher area weighted average organic carbon content values for agricultural soils calculated based on the BÜK200 than in the soil horizons of the FOCUS Hamburg soil scenario. This applies especially for the subsoils where the FOCUS Hamburg scenario provides a conservative setting with very low organic carbon contents. Furthermore, the organic carbon content analysis in the previous project based on the BÜK1000N (BGR 2007) showed a median organic carbon content of 1.6 % for the first soil horizon of all arable soils. Therefore, it can be suggested that the new soil database of the BÜK200, which has a higher spatial resolution, shows overall slightly higher organic carbon contents for the soils in areas with agricultural land uses.

Table 2: Area weighted average organic carbon contents of agricultural soils differentiated by depth (BÜK200, BGR 2017) in comparison to the FOCUS Hamburg soil scenario

Soil depth [cm]	Area weighted average org. carbon contents [%] BÜK200	Org. carbon content [%] FOCUS Hamburg
0-30 (with organic layers)	1.80	n.a.
0-30 (without organic layers)	1.73	1.5
30-60	0.50	1.0
60-75	0.62	0.2
75-90	0.48	0
90-100	0.11	0
60-100 (aggregated)	0.47	0.08
100-200	0.09	0

Table 3: Organic carbon contents of the FOCUS Hamburg soil scenario horizons and their corresponding spatial percentile according to nationwide soil data (BÜK200, BGR 2017)

Soil depth class [cm][1]	Organic carbon content [%] FOCUS Hamburg	Corresponding spatial percentile according to the BÜK200 [-]
0 - 30	1.5	31.9
30 - 60	1.0	95.9
60 - 75	0.2	66.8
75 - 90	0	0
90 - 100	0	0
100 - 200	0	0
0 - 100	0.78	60
0 - 200	0.39	74

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[1] The spatial percentile of the depth classes 0 – 30, 30 – 60, 60 – 75, 75 – 90, 90 – 100 and 100 – 200 cm relate to the spatial distribution of the area weighted C_{org} -average, the spatial percentile of the classes 0 – 100 cm and 0 – 200 cm relate to the spatial distribution of the depth weighted C_{org} -average

In Table 3 the spatial percentile of the organic carbon contents of the FOCUS Hamburg soil horizons in comparison to the nationwide distribution of the BÜK200 soils differentiated by depth classes is provided. In the first soil layer (0 – 30 cm) the Hamburg organic carbon content value represents a rather low percentile. Around 32 % of the agricultural soil area in Germany shows a lower organic carbon content in the upper soil layer. In the subjacent soil layer (30 – 60 cm) the opposite trend can be observed: Around 96 % of the agricultural soils are characterised by lower organic carbon content values compared to FOCUS Hamburg. The organic carbon content of 0.2 % in the FOCUS Hamburg subsoil in 60 – 75 cm depth corresponds to a spatial percentile of 67 % which means that 33 % of the agricultural soils are represented by lower organic carbon contents in this depth. All FOCUS Hamburg subsoil layers below 75 cm depth are defined with organic carbon contents of 0 %. The corresponding subsoil layers in the BÜK200 show the same ore higher organic carbon content values.

No clear tendency concerning the worst-case character of the organic carbon content parametrisation of the FOCUS Hamburg scenario in relation to the BÜK200 agricultural soils can be observed based on this analysis. Therefore, a spatial analysis of the depth weighted average of soil organic carbon was conducted both for the complete soil profile depth and a soil depth of 0 – 1 m.

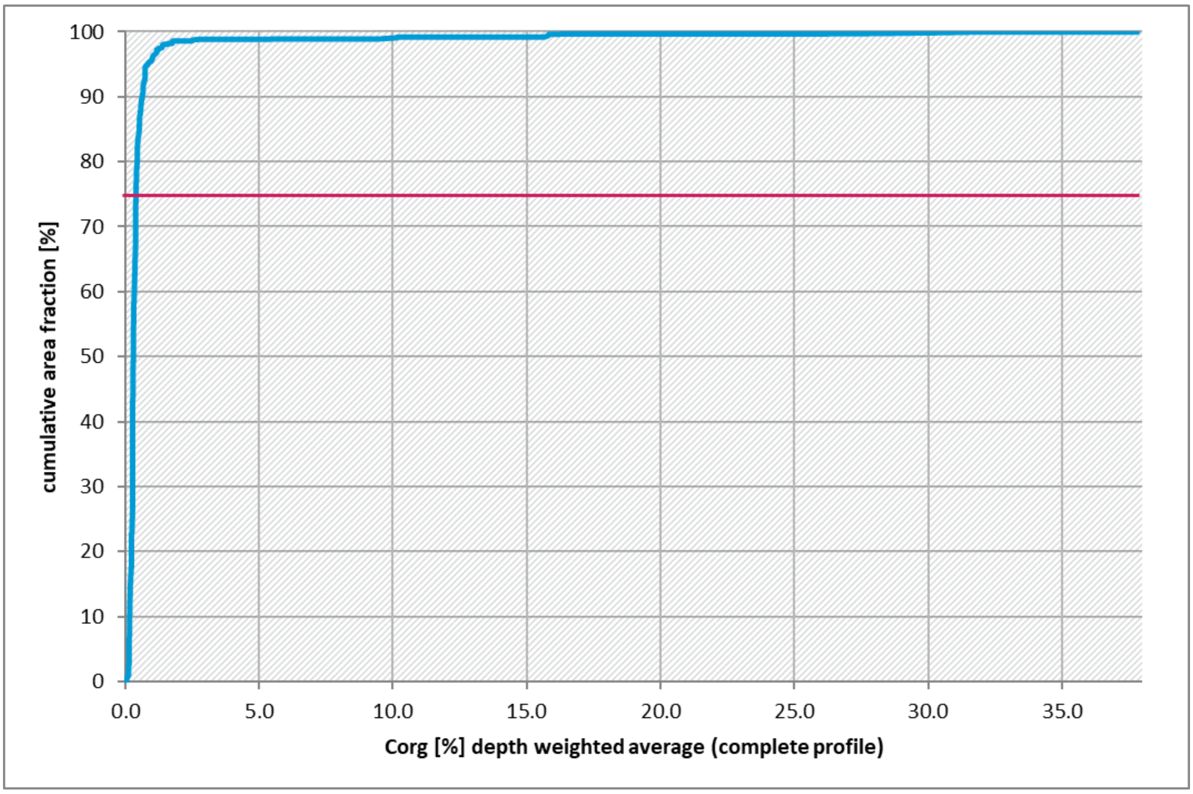
To calculate the depth weighted average organic carbon contents an organic carbon-depth-factor had to be generated for every soil horizon. The organic carbon contents of the soil horizons were multiplicated with the thickness of the soil horizons. The organic carbon-depth-factors were then summarized for each soil profile, and the result was divided by the thickness of the complete soil profile. Only soil horizons with a lower boundary equal or less than 1 m were included for the average calculation related to a soil depth of 0 to 1 m. In the last step a cumulative distribution function was generated for the depth weighted organic carbon content values (Figure 7).

The FOCUS Hamburg scenario is parameterised with a depth weighted average organic carbon content value of 0.39 % (0 – 200 cm) which corresponds to the 74th spatial percentile of the nationwide distribution of agricultural soils in Germany. Considering a soil depth of 1 m, which is conform to the standard leaching assessment for PPPs, a depth weighted average organic carbon content of 0.78 % was calculated. This corresponds to the 60th spatial percentile of the nationwide distribution of organic carbon contents for agricultural soils. That means that 60 % of the German agricultural soils are represented by lower depth weighted organic carbon contents compared to the FOCUS Hamburg scenario.

In the previous project the BÜK1000N (BGR 2007) in combination with soil data according to Düwel et al. (2007) and Utermann et al. (2009) were used to analyse the spatial distribution of the organic carbon soil contents (Klein et al. 2019b). Based on these evaluations the 1 m depth weighted organic carbon content of 0.78 % of the FOCUS Hamburg scenario meets the 73rd spatial percentile of nationwide soil data. These results indicate that the organic carbon contents of the BÜK200 (BGR 2017) are slightly higher than the values from the BÜK1000N, Düwel et al. (2007) and Utermann et al. (2009). Hence, it can be assumed that the use of the BÜK200 soil data base will slightly increase the spatial protection level of the FOCUS Hamburg scenario. The BÜK200/BÜK250 and the corresponding soil database according to BGR (2018a, 2018b) was used as suitable geodata to revise GeoPELMO DE.

Figure 7: Cumulative distribution function of the nationwide depth weighted organic carbon contents based on the BÜK200 compared to the FOCUS Hamburg scenario

The depth weighted organic carbon contents are related to complete soil profiles based on the BÜK200. The fuchsia colored line shows the corresponding depth weighted organic carbon content of the FOCUS Hamburg scenario as spatial percentile.



Source: own illustration, RLP AgroScience (according to BGR 2017)

4.2.1.2 Validation of measured organic carbon contents in arable subsoils

A realistic and conservative parametrisation of organic carbon contents in soils is crucial for spatial distributed leaching modelling for PPPs. Many subsoil horizons in the BÜK200 soil data base (BGR 2017) are characterised by a humus class 'h0' according to the BKA 5 (2005) and measured humus contents from laboratory analysis are not available. It was therefore critically discussed during the project if it is reasonable that the humus class 'h0' according to BKA 5 (2005) is specified by an organic carbon content of 0 %. Experts confirmed that it seems more realistic for agricultural soils that low organic carbon contents would still be measured in deeper subsoil layers. Therefore, the suggestion was made to use a value of 0.1 % or 0.2 % organic carbon content for all subsoil layers with the humus-class 'h0' for a nationwide soil scenario parametrisation of GeoPELMO DE.

A statistical analysis concerning the distribution of measured organic carbon content in deeper soil layers of arable soils was conducted to check this assumption based on a dataset containing analytical data of the permanent soil monitoring program of the Federal States. Based on this information the organic carbon contents in all humus classes h0 were validated. The dataset contains all together 4249 entry values of analytical results for the soil parameters carbonate content (TIC), carbon content (TC), organic carbon content (TOC) and humus content. Around 1900 soil horizon related values concerning the organic carbon and humus content were selected for further statistical evaluations. Finally, the 1900 analytical data points were again reduced to a number of 672 soil horizons for which a humus class of h0 was additionally identified in the field.

A depth related analysis was conducted with the remaining soil horizons. All measured organic carbon content values were arranged in ascending order concerning the soil depth where the samples were taken. For different depth classes some percentile values (10th, 30th and 50th percentile) and the arithmetic mean value were determined. Three classifications of different soil depths were used:

1. Depth classification according to the FOCUS Hamburg soil scenario: 0-30 cm, 30-60 cm, 60-75 cm, 75-90 cm, 90-100 cm, 100-200 cm
2. Depth classification in 20 cm steps: 0-20 cm, 20-40 cm, 40-60 cm, ..., 180-200 cm
3. Depth classification in 10 cm steps: 0-10 cm, 10-20 cm, 20-30 cm, ..., 190-200 cm

Table 4, Table 5 and Table 6 show the results of the statistical organic carbon content analysis separately for the different soil depth classifications. Only soil depth classes containing more than 10 data points have been included in the analysis and are provided down to a depth of 100 cm.

Table 4: **Results of the statistical organic carbon content analysis for the humus class h0 and depth classification related to the FOCUS Hamburg soil scenario [%]**

Soil depth [cm] n [-]	**30-60 128**	**60-75 99**	**75-90 86**	**90-100 28**	**60-100 weighted av.**
10th percentile	0.14	0.05	0.06	0.05	0.05
30th percentile	0.25	0.12	0.10	0.10	0.11
50th percentile	0.36	0.17	0.14	0.17	0.16
Arithm. mean	0.76	0.34	0.52	0.27	0.39

Table 5: **Results of the statistical organic carbon content analysis for the humus class h0 and depth classification in 20 cm steps [%]**

Soil depth [cm] n [-]	**20-40 40**	**40-60 93**	**60-80 122**	**80-100 91**	**60-100 weighted av.**
10th percentile	0.18	0.15	0.06	0.06	0.06
30th percentile	0.31	0.25	0.12	0.10	0.11
50th percentile	0.56	0.33	0.17	0.16	0.17
Arithm. mean	1.54	0.41	0.33	0.50	0.41

Table 6: **Results of the statistical organic carbon content analysis for the humus class h0 and depth classification in 10 cm steps [%]**

Soil depth [cm] n [-]	**30.5-40 35**	**40.5-50 48**	**50.5-60 45**	**60.5-70 74**	**70.5-80 48.**	**80.5-90 63**	**90.5-100 28**	**60-100 weighted av.**
10th percentile	0.15	0.16	0.15	0.05	0.08	0.06	0.05	0.06
30th percentile	0.30	0.26	0.23	0.12	0.11	0.10	0.10	0.11
50th percentile	0.56	0.33	0.39	0.19	0.16	0.15	0.17	0.17
Arithm. mean	1.67	0.43	0.39	0.31	0.35	0.61	0.27	0.39

Normally, the organic carbon contents in subsoil layers with a depth of 60-100 cm strongly decreases compared to upper soil layers. Consequently, the humus class h0 is more often allocated to subsoil horizons in the BÜK200 database. Because the organic carbon content parametrisation in the subsoils can impact the results of PELMO simulations, a closer look at this subsoil depth is crucial for the validation of the humus class h0 in the context of leaching modelling for PPPs:

Independently from the different soil depth classifications very similar percentile values for the measured organic carbon contents were calculated in a soil depth of 60 to 100 cm. The 10th percentile for the different classifications according to the FOCUS Hamburg scenario, in 20 cm steps and in 10 cm steps are 0.05 %, 0.06 % and 0.06 %, respectively. The 30th percentiles are always 0.11 %. The 50th percentile for the three calculation methods are 0.16 %, 0.17 % and 0.17 %, respectively. The arithmetic means are 0.39 %, 0.41 % and 0.39 %.

During the first advisory board meeting soil experts recommended to assume an organic carbon content value of 0.1 % for the humus class h0 in subsoils with arable land use. This value can be confirmed considering the 30th percentile values for the subsoils in 60 to 100 cm depth. The 30th percentile value represents a reasonable and conservative value to replace non-measured organic carbon contents with detected humus class h0 in field analysis. The use of an arithmetic mean value would be inappropriate because this value is distinctly higher (around 0.4 % organic carbon content) by the influence of outliers and therefore not conservative enough. Finally, this analysis provides evidence to define an organic carbon content of 0.1 % for the humus class h0 in subsoils with a depth of 60 to 100 cm for nationwide soil scenario definitions in PELMO according to the BÜK200 soil database (BGR 2017).

Since parts of the 672 C_{org} values available for the depth of 0 – 100 cm were aggregated values (more than 1 value at one depth at one measurement point) an advanced analysis of the original data without aggregated values was conducted. Around 800 organic carbon content single value measurements have been available for a soil depth of 0-100 cm with detected humus class h0 in the field. A 30th percentile value of 0.2 % organic carbon content was calculated for a soil depth of 0 – 60 cm, and a 30th percentile value of 0.1 % for a soil depth of 60 – 100 cm. These results confirm the analysis provided in Table 4, Table 5 and Table 6. Since organic carbon contents are apparently different in these two soil depths it was decided to use an organic carbon content value of 0.2 % for the humus class h0 in the soil depth 0 to 60 cm and 0.1 % for the humus class h0 in the soil depth 60 to 100 cm for nationwide soil scenario definitions and subsequent GeoPELMO DE simulations (see chapter 5).

4.2.1.3 Assignment of effective field moisture capacity and field capacity

The effective field moisture capacity, the field capacity and the permanent wilting point are required soil parameters for standard leaching modelling routines in PELMO considering chromatographic flow in the unsaturated zone. Those parameters are not always available as attribute data for the soil profiles in the BÜK200 database (BGR 2018a) and need to be derived from soil texture data. The information of horizon-specific soil types from the BÜK200 soil database were used to assign the effective field moisture capacity and the field capacity according to the published values in Dehner et al. (2015) and DWA (2016). Additionally, the permanent wilting point was calculated by subtraction of both values for each data point. Table 7 and Table 8 show the respective values. In contrast to previous values from the pedological mapping instruction (BKA 5 2005) there are substantial non-systematic discrepancies between these two documents and methods.

Table 7: **Used data of typical field capacities and effective field capacities based on soil texture data (Dehner et al. 2015, DWA 2016, translated into English)**

	Air capacity of soil [Vol%] water content at ME					**Field capacity [Vol%] water content at ME**					**Effective field capacity water content difference between ME und pF 4.2**					
Soil texture (German classification)	**Dry bulk density [g/cm^3] ****															**ME* pF***
	1.1	**1.3**	**1.5**	**1.7**	**1.9**	**1.1**	**1.3**	**1.5**	**1.7**	**1.9**	**1.1**	**1.3**	**1.5**	**1.7**	**1.9**	
Ss		40	32	24			11	12	13			9	10	11		1.9
St2		32	26	19	13		19	18	18	17		13	12	12	11	2.0
Sl3		27	22	15	10		24	22	22	20		15	13	12	10	2.0
Sl4		26	20	14	9		25	24	23	21		14	13	12	10	2.1
Slu		21	15	9	4		30	29	28	26		19	18	16	14	2.1
St2		35	28	21	14		16	16	16	16		10	10	10	9	2.1
St3		29	23	17	11		22	21	20	19		11	10	9	9	2.2
Su2		33	27	21	15		18	17	16	15		13	12	11	10	2.1
Su3		27	22	16	10		24	22	21	20		17	14	13	12	2.1
Su4		23	17	12	6		28	27	25	24		20	19	17	15	2.1
Ls2	24	18	13	7	3	35	33	31	30	27	19	17	15	14	11	2.1
Ls3	25	19	14	9	4	34	32	30	28	25	19	17	15	13	11	2.1
Ls4	29	23	18	12	7	30	28	26	25	23	17	15	13	12	10	2.1
Lt2	21	16	11	6		38	35	33	31		18	15	13	11		2.2
Lt3	16	11	8	4		43	40	36	33		18	15	11	9		2.3
Lts	23	18	13	8		36	33	31	29		16	13	11	9		2.2
Lu	22	16	12	6		37	35	32	31		19	17	14	13		2.2
Uu	24	17	11	6		35	33	33	31		26	24	24	21		2.1
Uls	26	19	14	8		33	32	30	29		21	20	18	16		2.1
Us	27	20	15	8		32	31	29	29		24	23	20	19		2.1
Ut2	25	18	11	5		34	33	33	32		23	22	22	21		2.2
Ut3	24	17	10	4		35	34	34	33		22	22	21	20		2.2
Ut4	22	16	10	4		37	35	34	33		21	19	18	17		2.2
Tt	10	6	3			49	45	41	-		13	12	9			2.5
Tl	15	10	6	3		44	41	38	33		14	13	9	7		2.5
Tu2	13	8	5	2		46	43	39	35		15	13	10	8		2.5
	Dry bulk density [g/cm^3] **															**ME***

	Air capacity of soil [Vol%] water content at ME					Field capacity [Vol%] water content at ME					Effective field capacity water content difference between ME und pF 4.2					
Soil texture (German classification)	**1.1**	**1.3**	**1.5**	**1.7**	**1.9**	**1.1**	**1.3**	**1.5**	**1.7**	**1.9**	**1.1**	**1.3**	**1.5**	**1.7**	**1.9**	**pF***
Tu3	15	11	8	4		44	40	36	33		18	15	11	8		2.4
Tu4	18	13	9	4		41	38	35	33		21	18	15	13		2.3
Ts2		15	10	8			36	34	29			11	9	7		2.4
Ts3		20	15	11			31	29	26			11	9	8		2.3
Ts4		23	19	14			28	25	23			12	10	9		2.2
fS, fSms, fSgs		36	28	20			15	16	17			12	13	14		2.0
mS, mSfs, mSgs		40	32	24			11	12	13			9	10	11		1.9
gS		42	34	27			8	9	10			6	7	8		1.9

*) Moisture equivalent in pF-values determined from water content measurements in the field at the beginning of the vegetation period using the pF-curve determined in the laboratory (see fig. 4, Renger et al. 2009)

**) In clay-rich soils, TRD of <1.1 g/cm3 may also occur at very low effective storage densities. In these rare cases, the LK, FK, and nFK are to be determined by extrapolation using the values given in Table 12.

In very humic topsoil substrates (especially Ap-horizons), information about the reduced dry bulk densities were considered to assign the effective field capacity and the field capacity. For pure peaty substrates in moors the categorisation in table 73 of the BKA 5 (2005) were used.

Table 8: Supplement values for pores (Dehner et al. 2015)

Soil texture (German classification) [-]	Total pore volume [Vol%]				Pores <50 µm (pF 1.8)				Pores <10 µm (pF2.5)				Pores <0.2 µm (pF4.2)			
	h2*	**h3**	**h4**	**h5**	**h2**	**h3**	**h4**	**h5**	**h2**	**h3**	**h4**	**h5**	**h2**	**h3**	**h4**	**h5**
Ss	2	4	7	15	3	5	10	20	2	4	8	17	1	2	4	7
St2	2	4	7	14	2	5	9	17	2	4	7	14	1	2	3	6
Sl3	2	4	8	15	2	4	9	16	2	3	6	13	1	1	3	5
Sl4	3	5	9	15	2	4	8	15	2	3	6	12	1	1	3	5
Slu	3	5	9	16	2	4	7	14	2	3	5	11	1	1	2	4
St2	2	4	8	14	2	5	10	17	2	4	8	14	1	2	3	7
St3	2	5	9	15	2	5	9	16	2	4	7	13	1	2	3	6
Su2	2	4	8	15	2	5	10	18	2	4	7	14	1	2	3	6
Su3	2	5	9	15	2	5	9	16	2	4	7	13	1	2	3	5
Su4	2	5	8	15	2	5	8	15	2	4	6	12	1	2	2	5

Soil texture (German classification) [-]	Total pore volume [Vol%]				Pores <50 µm (pF 1.8)				Pores <10 µm (pF2.5)				Pores <0.2 µm (pF4.2)			
	h2*	h3	h4	h5	h2	h3	h4	h5	h2	h3	h4	h5	h2	h3	h4	h5
Ls2	3	6	9	16	2	4	7	13	1	3	5	10	1	1	2	4
Ls3	3	5	9	16	2	4	7	14	2	3	5	11	1	1	2	4
Ls4	3	5	9	15	2	4	8	14	2	3	6	11	1	1	2	4
Lt2	3	5	9	16	2	3	6	11	1	2	4	9	0	1	2	3
Lt3	3	6	10	17	1	3	6	11	1	2	4	9	0	1	2	3
Lts	3	6	10	17	2	4	7	13	2	3	5	10	1	1	2	3
Lu	3	5	9	16	1	3	6	11	1	2	4	9	0	1	1	3
Uu	1	4	7	14	1	3	5	10	1	2	4	8	0	1	2	3
Uls	3	6	9	16	2	4	6	12	1	3	4	10	0	1	2	3
Us	2	5	8	15	2	4	6	12	1	3	4	10	0	1	2	4
Ut2	3	6	10	16	2	4	7	11	1	3	5	9	0	1	2	3
Ut3	3	6	11	17	2	4	7	11	1	3	5	9	0	1	2	3
Ut4	4	7	11	16	2	4	7	10	1	3	5	8	0	1	2	3
Tt	4	6	9	15	1	2	4	8	1	1	3	6	0	1	1	2
Tl	3	6	9	14	1	2	4	8	1	1	3	6	0	1	1	2
Tu2	3	6	9	15	1	2	4	8	1	1	3	6	0	1	1	2
Tu3	3	4	9	15	1	2	5	8	1	1	4	6	0	1	1	2
Tu4	3	5	9	16	1	2	5	9	1	1	4	7	0	1	1	2
Ts2	4	6	11	18	2	3	7	13	1	2	5	10	1	1	2	4
Ts3	3	6	11	18	2	4	8	14	2	3	6	11	1	1	2	4
Ts4	3	6	10	17	2	4	8	14	2	3	6	11	1	1	2	4

* With increasing humus content, the dry bulk density decreases or the total pore volume of the soil increases. Therefore, it must be considered with the humus supplements that at high humus contents correspondingly lower dry bulk densities are present.

Table 9: Reduced soil bulk density for high humus contents

Humus class (German classification	Dry bulk density class [-]	Humus mass [%]	Dry bulk density [g/cm^3]	Pure density [g/cm^3]	Total pore volumes [Vol.-%]
h3	<= 3 (4)	3	<1.70	2.59	>34
h4	<= 3	6	<1.55	2.53	>39
h5	<= 1 (2)	11,5	<1.20	2.42	>50

4.2.2 Climate data

Information from the National Meteorological Service in Germany (DWD, Deutscher Wetterdienst) was considered for the implementation of climate data in GeoPELMO DE. Altogether 299 weather stations (DWD 2012) were selected with available data on daily temperature, relative humidity and precipitation data for the period 1985 - 2010 (26 years include 6 ´warming up´ years and 20 years for PEC modelling). The implementation of those daily weather data for the period 1985 - 2010 corresponds to the FOCUS leaching modelling approach for PPPs in Europe (European Commission 2014). The same climate data were already used in the first GIS version of PELMO (Klein et al. 2019b). Daily evapotranspiration data were only available for a selected number of these weather stations. 50 weather stations with missing evapotranspiration data were completed by the data of the station with the shortest spatial distance. The list of DWD stations with substitution of evapotranspiration data is published in section 3.3.5 in Klein et al (2019b).

The spatial assignment of the 299 selected weather station data to the German agricultural area in GeoPELMO DE is based on a statistical analysis with raster datasets from Germany´s National Meteorological Service with monthly average values of temperature and precipitation for the climate period 1980 – 2009 and a spatial resolution of 1 x 1 km (DWD, 2012) (Klein et al. 2019b). From these DWD raster datasets seasonal average temperature and precipitation values were derived for the period 1980 – 2009 and compared to seasonal average temperature and precipitation values of each weather station. The shortest Euclidian distance of both combined parameters (see equation below) was finally used to assign all weather stations to the raster dataset of the agricultural area defined in GeoPELMO DE. This spatial assignment was limited to the three major hydrogeologic regions in Germany according to map 5.1 of the Hydrogeologic Atlas of Germany (HAD). The analysis is based on the calculation provided in Klein et al. (2019b, p. 120):

$$Diff_{i,j,k} = \sum_{JZ=1}^{4} \left((Temp_{JZ,i,j} - Temp_{JZ,k})^2 + (NS_{JZ,i,j} - NS_{JZ,k})^2 \right)$$

$Diff_{i,j,k}$: cumulative difference of raster cell (i,j) from the weather station k

$Temp_{JZ,i,j}$: mean temperature of raster cell (i,j) during season JZ

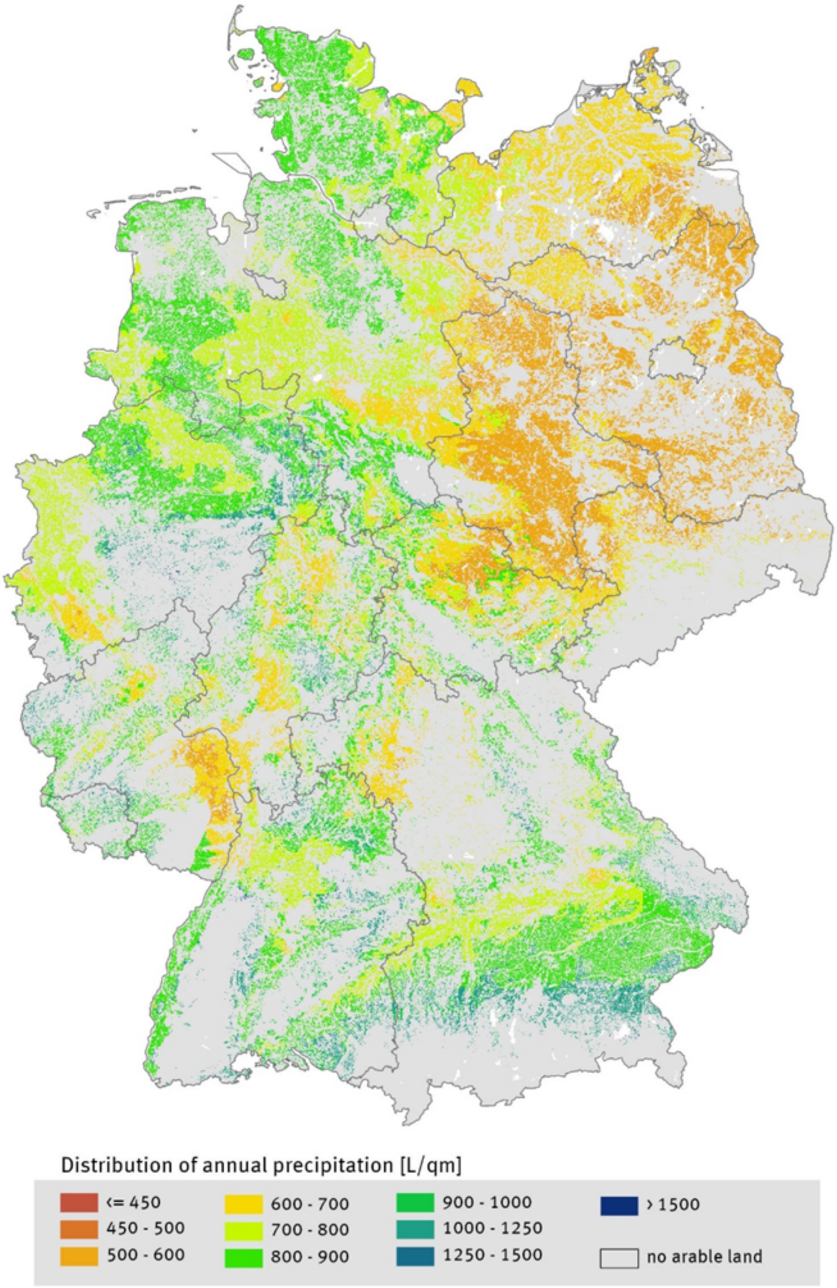
$Temp_{JZ,k}$: mean temperature of station k during season JZ

$NS_{JZ,i,j}$: mean precipitation of raster cell (i,j) during season JZ

$NS_{JZ,k}$: mean precipitation of station k during season JZ

After the analysis and assignment of 299 DWD stations to the agricultural area in Germany the map basis for the agricultural area was resampled to a raster dataset with a resolution of 200 m x 200 m to match the resolution of the BÜK250 soil map (BGR 2018b) (see Figure 8). Based on this spatial map resolution in GeoPELMO DE the average precipitation distribution in Germany with generally higher rain amounts in the Western part and lower rain amounts in the Eastern part is provided in Figure 8.

Figure 8: **Distribution of 20 years averaged precipitation [mm] in GeoPELMO DE 2.0 (1991 – 2010) according to DWD (2012)**



Source: own illustration, Fraunhofer IME

4.3 Macropore flow/preferential flow

The implementation of preferential flow in a nationwide version of PELMO requires a general development of adjusted modelling routines and their adaption to numerous soil-climate scenario which represent national environmental conditions. It was already discussed in section 3.2 that quantifying the degree of preferential PPP-transport occurring through different soils as an outcome of variable changing climatic conditions can a be challenge (Berg et al. 2014). Shrinkage cracks appearing in clayey soils during dry weather periods, bio-pores in the soil rootzone and caused by earthworm activities as well as vertically oriented inhomogeneities of the geological substrate or fractured media like fractured glacier clayey tills, limestones and solid rocks are scientifically discussed as causes which can generate hydraulic active discontinuities influencing the water balance and substance flow and transport in the unsaturated zone (Haarder et al. 2021, Klint et al. 2004, Rosenbom et al. 2008, Wessolek 2004). Besides, the depths and fluctuating groundwater tables additionally influence those processes.

It was discussed with experts in the advisory board of the project that considering all causes for preferential flow and their spatial and temporal characteristics in a scientific sound classification would be difficult, because scientific knowledge and nationwide information and geodata are sometimes not available. Criteria for earthworm activity and bio-pore intensity, for example, would be available from the literature and pedo-transfer functions could be used, however, data are still missing to come up with a nationwide classification system. However, there was also consensus in the advisory board that missing scientific information or missing geodata should not lead to a non-consideration of preferential flow in the development of a spatial distributed models, because this could even lead to higher underestimation of pesticide leaching for certain areas under certain weather conditions. It was suggested by the experts that a simple soil classification could be developed for the implementation of a new modelling routine related to preferential flow.

A soil macropore classification was finally developed which considers the texture and very high humus contents of the soils as well as the occurrence of near-surface groundwater tables (section 4.3.1). The classification mainly represents the vulnerability of soils to develop and preserve desiccation cracks under dry weather conditions. The tendency of the soils to conserve bio-pores over time is partly covered with that classification. It was decided to apply the overall soil classification for macropore vulnerability to a soil profile depth of 1 m based on the soil data from the BÜK200/BÜK250 soil data base (BGR 2018a, 2018b).

Different geodata were discussed during the project. Because soil characteristics are directly based on the geological parent material and/or its rock base, the lithography of sediment and rock types based on the General Hydrogeological Map of Germany with a scale of 1:250.000 (HÜK250, BGR 2024) could be alternative geodata for a soil macropore classification. The hydraulic conductivity data from the HÜK250 could be used in association with the lithography data, because soils with a higher portion of fine substrates generally provide a lower conductivity. Hence, this parameter correlates with soils and substrates which have different vulnerabilities to develop macropores by drying shrinkage. However, both data layers from the HÜK250 are not provided for different soil depth. It was finally decided to use the soil data from the BÜK250 to be consistent with the implementation of other processes (e.g. runoff, soil organic carbon contents).

The model FOCUS PELMO simulates chromatographic flow in the unsaturated soil zone and parameters to calculate preferential flow were not defined for PELMO by FOCUS (2000). However, FOCUS PELMO includes a simple preferential flow module which was developed within the EU financed research project APECOP (Vanclooster et al. 2003) and tested against the results of lysimeter studies (Klein et al. 2019a). Two alternative approaches, the reduction of field capacity and the increase of the dispersion length in soil, are additional available which lead also to an increasing transport velocity of water and chemical substances through the soil profile. The three different technical possibilities in PELMO to account for preferential flow are compared and explained in section 4.3.3 in more detail. It was further decided during the project to calibrate or validate the new modelling routine preferential flow in PELMO on available monitoring data of pesticides for the different soils. The evaluation of monitoring data to quantify preferential flow for PPPs in GeoPELMO DE is provided in section 4.3.4.

4.3.1 Macropore classification for agricultural soils in Germany

The final algorithm to classify all agricultural soils to their potential to develop macropores is provided in Figure 9 and explained in more detail in the following subsections. The classification follows a weighting approach of the soil horizon data provided in the BÜK200 /BÜK250 soil data based by its texture and humus content (line 1-3 in Figure 9) (BGR 2018a, 2018b). Each soil profile used in GeoPELMO DE is finally assigned to one of the three remaining soil classes. Although a different range of the calculated weighting macropore factor (described as ´weightes macropore classes´ in line 5 in Figure 9) is used for the final soil profile classification in three different classes (line 7 in Figure 9):

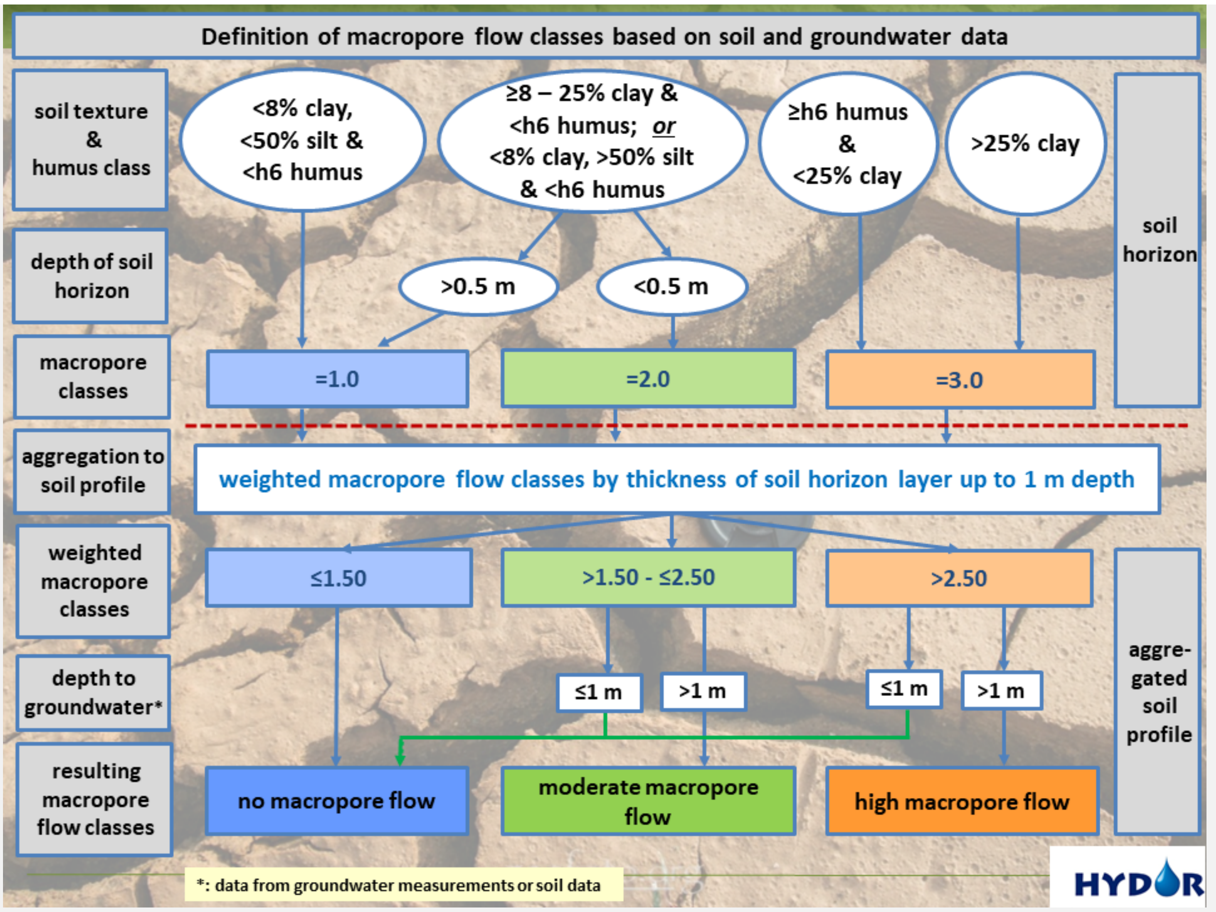
≤ 1.50 = no macropore/preferential flow

> 1.50 - ≤ 2.50 = moderate macropore/preferential flow

> 2.50 = high macropore/preferential flow

Figure 9: Final algorithm to define macroporosity (macropore classes)

The algorithm is developed for available soil data from the German soil database from BÜK200/ BÜK250.



Source: own illustration, HYDOR (according to BGR 2018a, 2018b)

4.3.1.1 Influence of soil texture on macropore classes

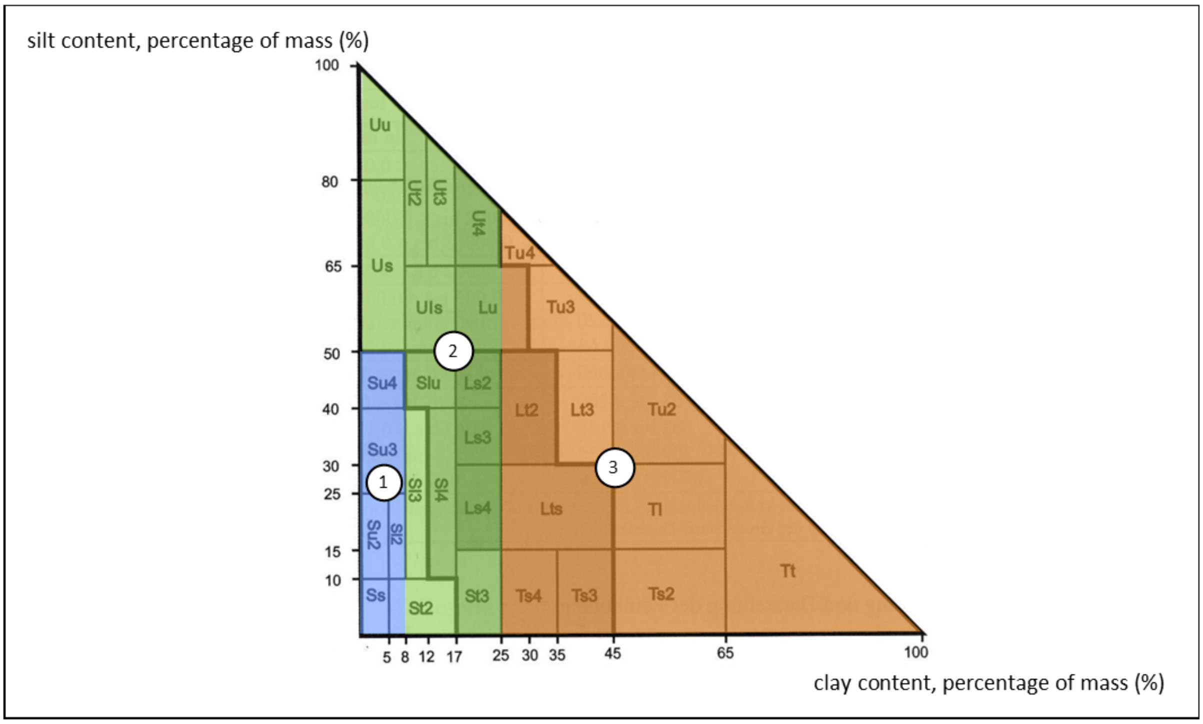
To classify the vulnerability of different soil types in Germany according to their potential to develop macropores, the tendency of each soil horizon from the BÜK200/ BÜK250 data base (BGR 2018a, 2028b) to form desiccation cracks in coherent substrates by shrinkage is considered by a simple texture classification. Silt and clay mass percentages and the resulting soil types according to the German soil mapping guideline BKA 5 (2005) were used in a first classification of the available soil horizons. With increasing clay content, a higher vulnerability to develop macropores is assumed.

Macropore horizon class 1 contains mainly sandy soil layers like pure sands, loamy and silty sands that feature a clay content less than 8 %. Macropore horizon class 2 represents soil layers with a clay content between 8 % and 25 %. Loamy silts and sandy loams, amongst others, are additional allocated to class 2. Horizon class 3 comprises soil layers with a clay content higher than 25 % like clay rich loams, clay rich silts and loamy clays (line 1-3 in Figure 9, Figure 10).

The analysis is limited to dominant soil profiles for the land uses arable fields and permanent crop as well as up to a maximum soil depth of 1 m below surface. This results in a first classification of 4285 soil horizons from the BÜK200 /BÜK250 soil database.

Figure 10: Silt and clay mass percentage to classify soil horizons to their texture and vulnerability to develop macropores

The soil texture classes are related to the German soil mapping guideline BKA 5 (2005).



Source: own illustration, HYDOR

4.3.1.2 Influence of organic carbon content on macropore classes

It was decided to consider soils very rich in humus in the macropore classification because high contents of organic matter can lead to macropore development in such soils in very dry seasons. Table 10 shows the official classification of humus contents in soils according to the German soil mapping guideline BKA 5 (2005), which was used to classify the soil horizons available in the BÜK200 soil database. Finally, only soil horizons with humus class h6 and h7, which represent extremely humic soils and peats with more than 15 mass percent humus (e.g. the German soil type 'HN' = low-level moor peat), are considered in the classification to develop macropores due to shrinkage.

Table 10: Humus-classes based on mass percent of humus (BKA 5 2005)

Humus (organic part)		
Class [-]	**Description [-]**	**Mass percent [%]**
h0	no humus	0
h1	very weakly humic	<1
h2	weakly humic	1 - 2
h3	moderately humic	2 - 4
h4	strongly humic	4 - <8
h5	very strongly humic	8 - <15
h6	extremely humic (half-bog)	15 - <30
h7	organic peat	>=30

4.3.1.3 Influence of depth of soil horizon on macropore classes

In the applied classification scheme an overall soil depth down to 1 m below surface was considered only. Soil horizons below 50 cm in depth are assumed to have a higher soil moisture due to its lower distance to the groundwater table. Therefore, soil horizons below 50 soil depth, which are normally classified by its texture and/or humus content in macropore class two (>= 8-25 % clay and/or >= h6, or < 8 % clay and > 50 % silt and < h6), are assigned to class one without macropores (Figure 9, second and third line). Due to present adhesive water in more cohesive soils, it is not assumed that soils with higher clay contents and extremely humic soils build up a layered differentiation down to a soil depth of 1 m. Therefore, that adjustment of a different soil depth was not considered for soil horizon classification in class three (> 25 % clay or < 25 % clay and >= h6).

4.3.1.4 Aggregation of soil horizons to a soil profile macropore classification

The first step of the soil vulnerability classification to macropores development is based on individual soil horizon data which can lead to different macropore classes for the horizons in one single soil profile. The technical implementation in PELMO requires an aggregation of the horizon classes and to obtain only one characteristic macropore class for each soil profile. A simple weighting approach for all horizons down to 1 m soil depth was therefore applied. Horizons which exceed 1 m soil depth (e.g., a horizon starts at 70 cm depth and ends at 130 cm depth) were only taken into account by its part down to 1 m. The defined macropore class numbers of the soil horizons were weighted by their depths in relation to the 1 m soil profile. As a result, a macropore classification number was calculated for each soil profile in the BÜK200/ BÜK250 data base according to BGR (2018a, 2018b) (Figure 9, Table 11).

This classification method can lead to uncertainties of the depth-related macropore vulnerability for single soil profiles. This was observed in a few cases, e.g. predominantly in soils where sandy horizons overlie horizons with high organic contents. These soils would be less vulnerable to desiccation cracks on the surface due to its sand content. By weighting, the underlying organic horizons increase the overall vulnerability (classification number) of these soil profiles to develop macropores. An evaluation of these few cases with minor occurrence in Germany shows only an insignificant impact to the overall macropore classification for the agricultural area. The simple weighting process was therefore regarded as applicable.

The classification method and the weighting of soil horizons to calculate a macropore class for each soil profile is visualized in Table 11 by four soil profile examples. The used colour scheme for the different classes is comparable to Table 12.

Table 11: Examples of weighting macropore classes of soil horizons to single soil profiles

Soil ID [-]	Soil profile type [-]	Soil horizon type	Depth of horizon from [cm]	Depth of horizon to [cm]	Soil horizon thickness [cm]	Humus class [-]	Initial macropore class [-]	Macropore class adjusted by depth [-]	Weighted macropore class for entire soil profile [-]
30	MC	Ut4	0	25	25	h3	2	2	moderate (1.7)
30	MC	Ut4	25	79	54	h0	2	1	
30	MC	Tu4	79	100	21	h0	3	3	
56	RZ	Lt2	0	23	23	h5	3	3	moderate (1.6)
56	RZ	Sl4	23	35	12	h1	2	2	
56	RZ	Su3	35	100	65	h0	1	1	
72	SS	Sl3	0	30	30	h3	2	2	no (1.3)
72	SS	Sl2	30	40	10	h1	1	1	
72	SS	Ls3	40	100	60	h0	2	1	
177	GM	Sl3	0	25	25	h4	2	2	no (1.3)
177	GM	Sl3	25	40	15	h6	3	3	
177	GM	Su2	40	75	35	h0	1	1	
177	GM	Sl3	75	100	25	h0	2	1	

Table 12: Colour scheme for the different vulnerability classes

Vulnerability class	Macropore class
no macropore flow	<= 1.50
moderate macropore flow	>1.50 - <=2.50
high macropore flow	>2.50

4.3.1.5 Influence of depth to groundwater on macropore flow classes

In the last step of the macropore classification all agricultural soils influenced by very shallow groundwater were assigned to the soil class with no macropore flow (last line in in Figure 9).

Areas with a groundwater table depth less than one meter were applied for this adjustment. No vulnerability to macropore development due to desiccation is assumed in those agricultural areas.

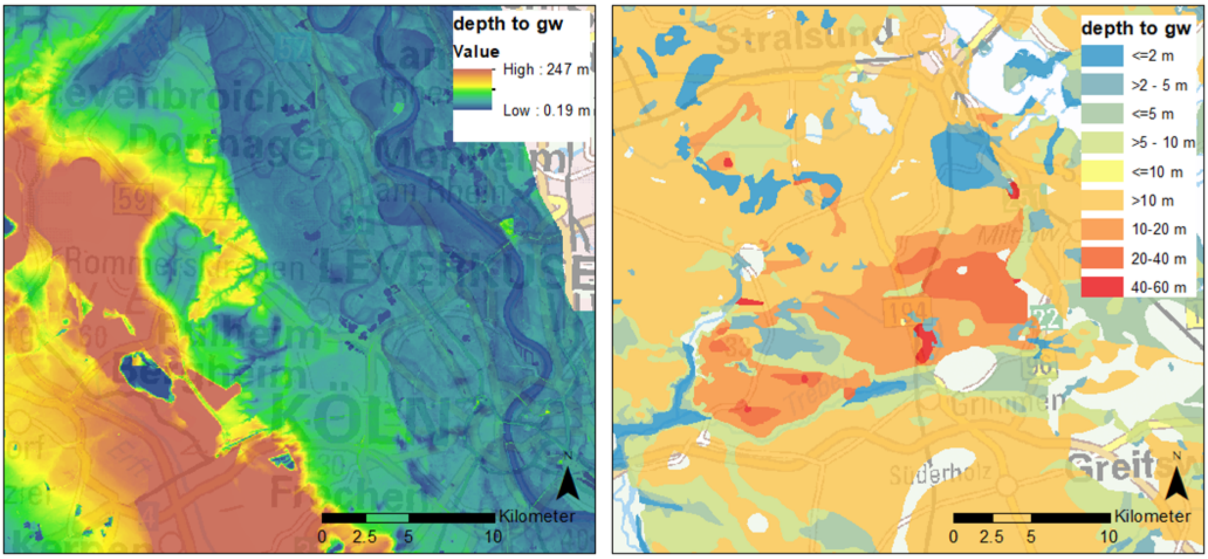
Table 13: Availability of groundwater table depth data in different Federal States of Germany

Federal states	Government agency	Available data	Data type
Schleswig-Holstein	LLUR	Area-wide (90% coverage) mean lowest groundwater level below surface (MNGW) BÜK200	categorized polygon data
Mecklenburg-West Pomerania	LUNG	Area-wide mean depth to groundwater table	categorized polygon data
Brandenburg	LfU BB	Area-wide mean depth to groundwater table	categorized polygon data
Lower Saxony	LBEG	Area-wide mean lowest/ mean highest groundwater level below surface (MNGW/ MHGW) BK50	categorized polygon data
North Rhine-Westphalia	LANUV NRW	Depth to groundwater table data, only around 55% coverage	continuous raster data
Saxony-Anhalt	LHW	Area-wide depth to groundwater table data	continuous raster data
Saxony	LfULG	Depth to groundwater table data, only 80% coverage	categorized polygon data
Thuringia	TLUG	Area -wide depth to groundwater table data, but only class < 2m	categorized polygon data, only one single class (<2m)
Hesse	HLNUG	Area-wide depth to groundwater table data	continuous raster data
Baden-Württemberg	LUBW	Depth to groundwater table data available only for small regions (Rhine Rift & small other areas)	continuous raster data
Rhineland-Palatinate	LfU RLP	no depth to groundwater table data available	no data
Bavaria	LfU BY	no depth to groundwater table data available	no data
Saarland	LfU SL	no depth to groundwater table data available	no data

Data about the groundwater table depth were available for most of the Federal States in Germany. Unfortunately, these data are not consistent, because some Federal States provided detailed raster data and others provided categorized data, only. The categorized data were in some cases from lower precision, because the lowest class on groundwater depth was aggregated to two meters. In those cases, the assignment of the soils and sites to the class with no macropore flow was conducted when the groundwater table occurs at two meters instead of the intended one meter. Table 13 lists the availability and quality of depth to groundwater table data in different Federal States during the project. No data was available for the Federal States Bavaria, Rhineland-Palatinate and Saarland.

Figure 11 illustrates a comparison of two different data types, which were available: In North Rhine-Westphalia, area-wide, continuous depth to groundwater table data were provided as raster data. For Mecklenburg-West Pomerania, pre-processed categorized data in polygon maps were available, which are from less accurate spatial and depth-related resolution. Figure 12 and Figure 13 additionally demonstrate the area-wide available depth to groundwater data in Brandenburg and Saxony-Anhalt.

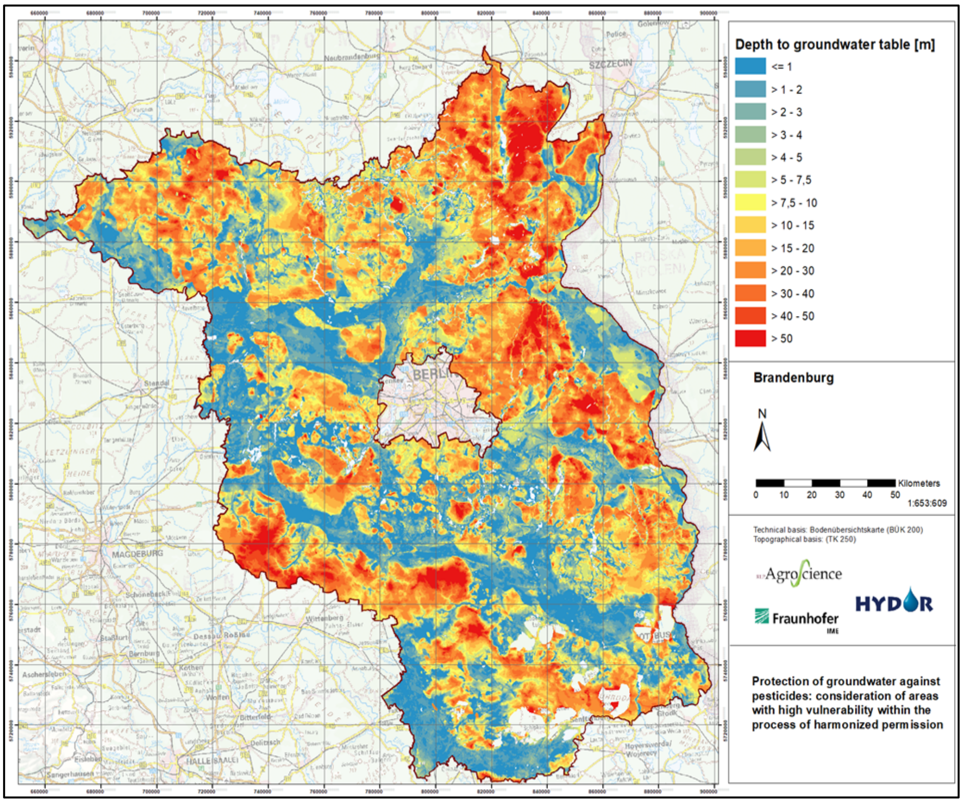
Figure 11: Spatial distribution of different available depth to groundwater table data in North Rhine-Westphalia (left, raster based) and Mecklenburg-West Pomerania (right, categorized)



Source: own illustration, HYDOR

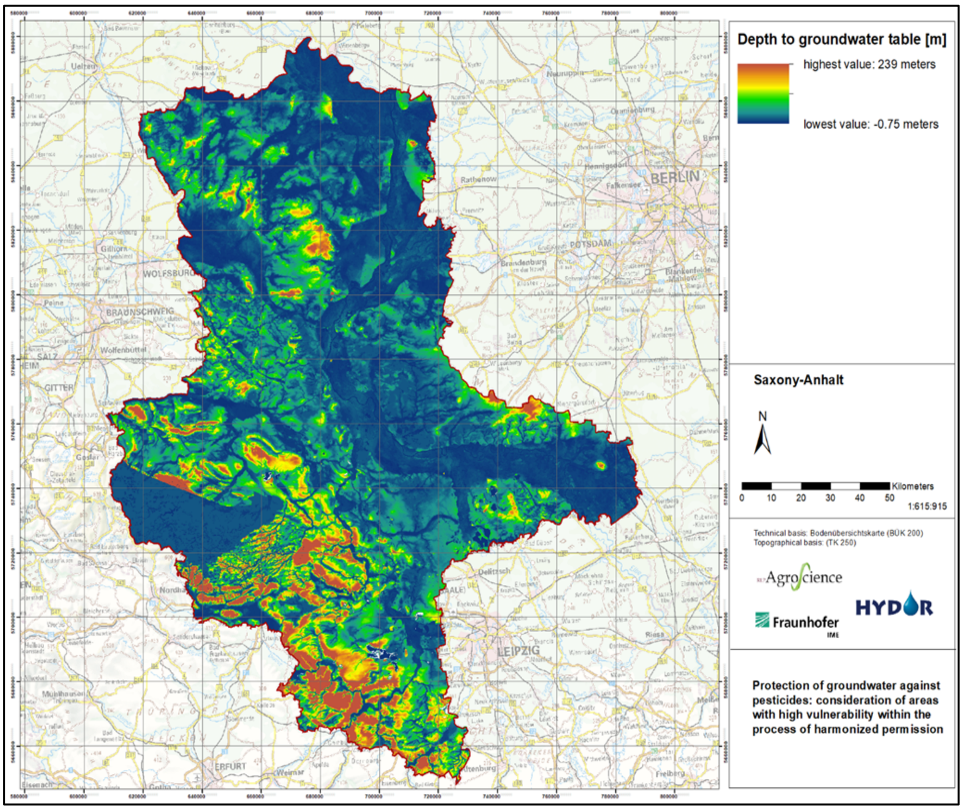
For the Federal States where no depth to groundwater table data were available, alternative solutions were applied. The BÜK200 (BGR 2018a) and BK50 (soil map with a scale of 1:50.000) both comprise data for highest and lowest mean depth to groundwater table. However, the coverage of the data from the BÜK200 is very sparse. Therefore, soil data from the BÜK200 were only used in Schleswig-Holstein as an alternative data source. Figure 14 demonstrates the spatial distribution of available groundwater data (mean lowest depth to groundwater = MNGW) from the BÜK200 in Schleswig-Holstein when they are clipped to the agricultural area represented by arable fields and permanent crops. Since a depth to groundwater ≤ 1 m is assumed to adjust soils to the class of no macropore flow, the two classes ≤ 0.4 m (blue colour in Figure 14) and 0.4 - 0.8 m (dark green colour in Figure 14) were used in Schleswig-Holstein for this adaption. Data from the BK50 with a better resolution compared to the BÜK200 were only available for Lower Saxony. Figure 15 shows the spatial distribution of available groundwater table depth data (MNGW) for Lower Saxony. To achieve the best possible data base, the depth to groundwater was partially complemented with values from the mean highest depth to groundwater (MHGW) when the mean lowest depth to groundwater (MNGW) was not available. Large areas in Northern Lower Saxony (blue colour in Figure 15) could be potentially adjusted to the soil class with no macropore flow. It must be considered that a clipping to the agricultural area was not yet performed in Figure 15 for the data overview.

Figure 12: Area-wide spatial distribution of available depth to groundwater data in Brandenburg (categorized data)



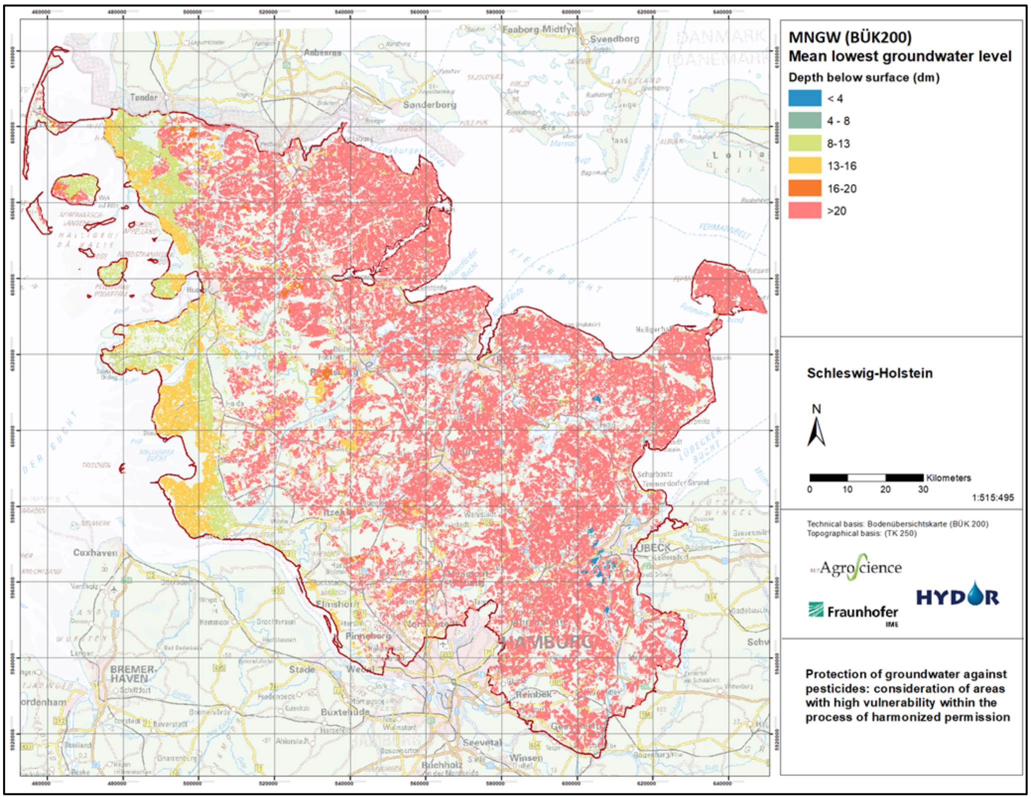
Source: own illustration, HYDOR

Figure 13: Area-wide spatial distribution of available depth to groundwater data in Saxony-Anhalt (raster-based data)



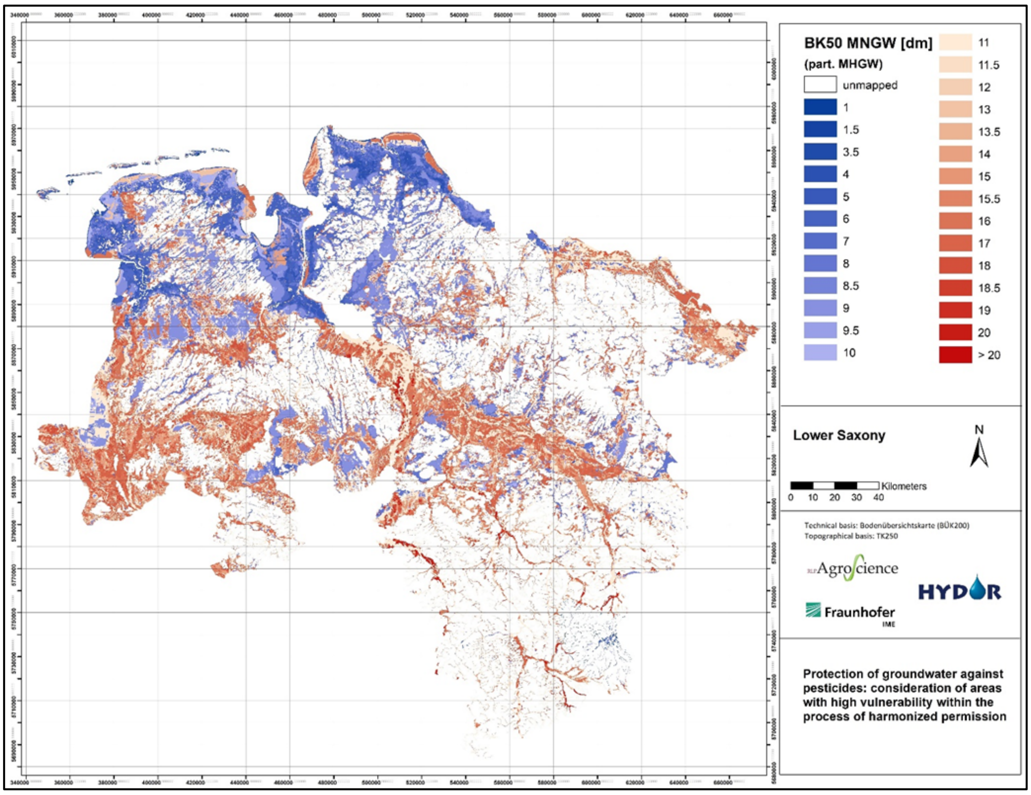
Source: own illustration, HYDOR

Figure 14: Spatial distribution of available BÜK200 groundwater table depth related data (MNGW) in Schleswig-Holstein



Source: own illustration, HYDOR (according to BGR 2018a)

Figure 15: Spatial distribution of available BK50 groundwater table depth related data (MNGW/MHGW) in Lower Saxony



Source: own illustration, HYDOR

In the project, only hydrological data in agricultural areas was used for the macropore classification. An adjustment by soil types based on the BÜK200 data was discussed as possible approach for all other areas or Federal States with missing data on the groundwater table depth. In those cases, a shallow depth to the groundwater table ≤ 1 m could be assumed for the soils A-type (floodplain/wetlands) and G-type (gley). However, in some of those areas, a higher portion of the agricultural area would be adjusted to the class without macropore flow with that method, because not all areas with floodplain, wetlands or gley soils are necessarily influenced by a groundwater table lower than one meter. Floodplain, wetlands (A-type) or gley (G-type) soils occur in the middle part of the map whereat the half of those soils occur in the eastern part of the map in an area with a groundwater table deeper than 1 m. As a consequence, an adjustment to the class without macropore flow for all soil types A or G would introduce uncertainties. It was therefore decided to omit the last adjustment step in the classification scheme for areas where groundwater table depth data was not available (Bavaria, Rhineland-Palatinate and Saarland). The overall nationwide impact on the soil macropore classification is expected to be rather small.

4.3.2 Spatial distribution of soil vulnerability to develop macropores in agricultural areas in Germany

The final step of the macropore classification, the adjustment by groundwater table depth, can lead to different macropore classes for the same soil profile (soil ID) in different areas with different groundwater depth. To compensate this for the technical implementation in GeoPELMO DE, an evaluation of areas with the same soil ID adjusted by groundwater table depth in relation to the overall area of this soil IDs was performed. Only the dominant macropore class, which finally characterises the major area of this specific soil ID (> 50 % of the area), was further used for the scenario definition in GeoPELMO DE.

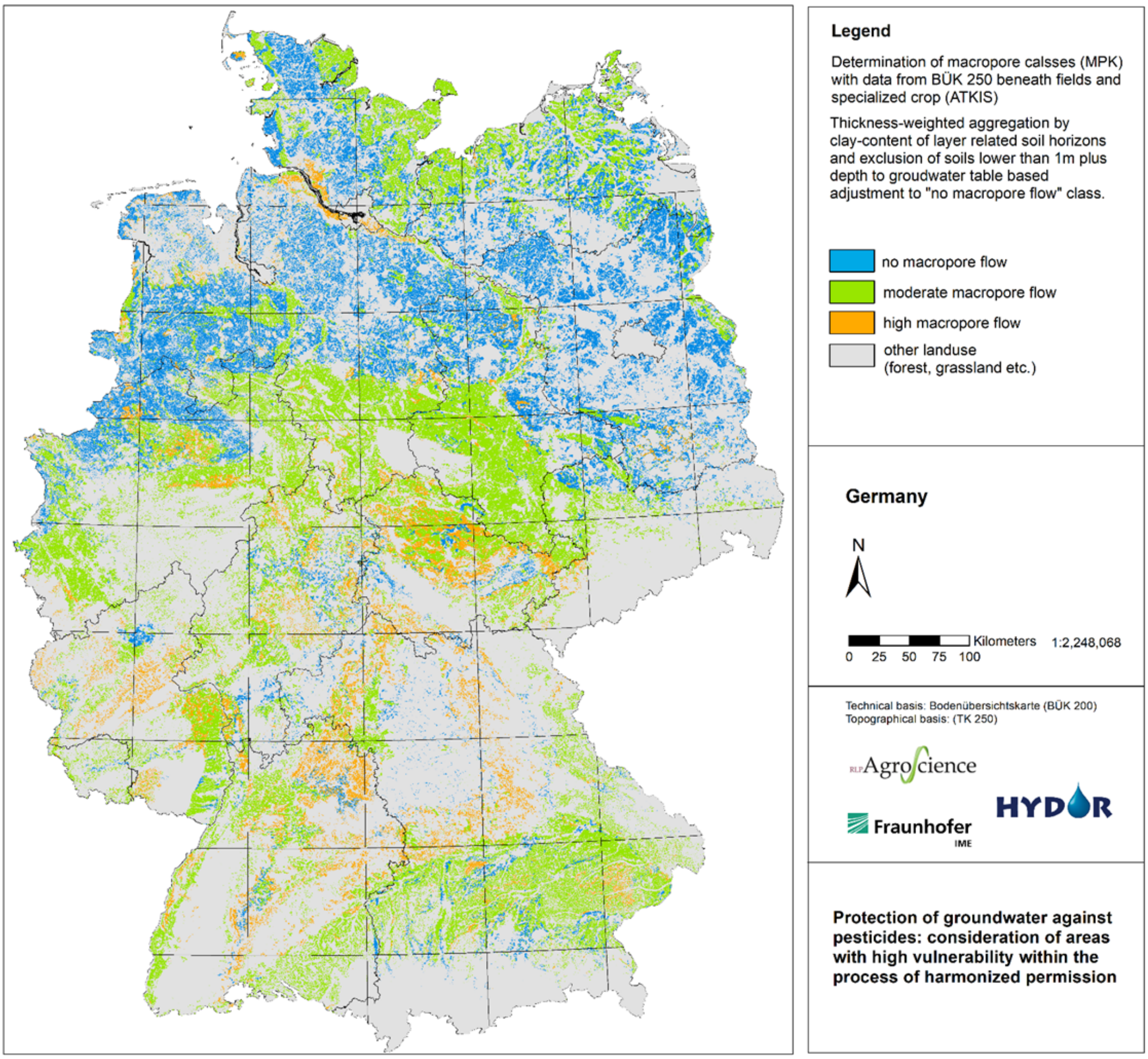
The final distribution of three soil macropore classes for the agricultural area in Germany is provided in Figure 15 according to the classification scheme in Figure 9. Finally, 34.8 % of the German crop land is classified without a tendency to macropore flow, 25.9 % of arable fields have a potential to moderate macropore flow and 12.3 % to high macropore flow (see Table 14). Clearly visible is a demarcation between soils of the two classes 'no macropore flow' and 'moderate macropore flow' in the northern part of Germany. Highly permeable sandy soils primarily occur in ancient morainal plains and river valleys in Northern Germany (e.g. large areas in the southern land ridge), which are classified not to develop macropores. Agricultural soils originated from glacier tills are classified to 'moderate macropore flow' (see the very northeastern part of Germany in

Figure 17). Furthermore, the middle river valley of the Elbe contains soils with 'moderate macropore flow'. Soils classified with a high potential to develop macropore flow are located further down-stream in the Elbe River valley. They are characterized by substrates with moderate hydraulic conductivity, which often consist of fine sands and silty sediments. At the eastern border of Brandenburg, the Oderbruch is predominantly characterised by cohesive soils which facilitate the formation of macropores and are therefore classified by 'moderate macropore flow'.

In the Thuringian Basin (see

Figure 17), a higher portion of cohesive soils is present which are classified in both soil macropore classes 'moderate macropore flow' and 'high macropore flow'. Those soils occur in areas with different Triassic sediments of limnic, coastal or marine origin (e.g., from the Keuper), which are characterised by different hydraulic conductivities. Soils classified with 'no macropore flow' are mainly located in quaternary sediments, mostly in bench gravels with a high hydraulic conductivity.

Figure 16: Spatial distribution of soil macropore classes in Germany

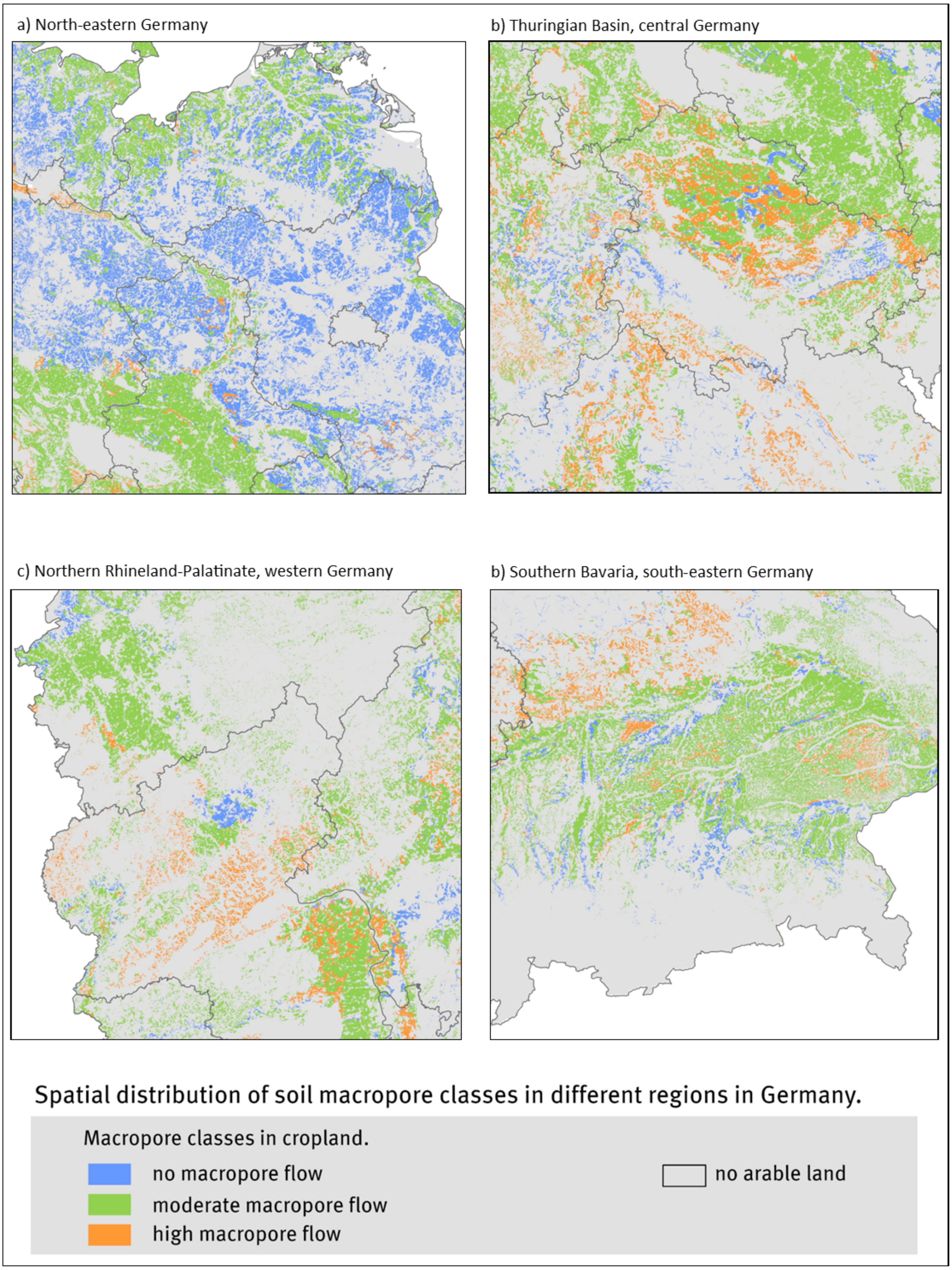


Source: own illustration, HYDOR

Table 14: Area fractions of macropore classes for cropland in Germany.

macropore class [-]	Arable area [km^2]	Arable area [%]
no macropore flow (1)	38378	34.8
moderate macropore flow (2)	58218	52.9
high macropore flow (3)	13523	12.3

Figure 17: **Spatial distribution of soil macropore classes in different regions in Germany.**



Source: own illustration, HYDOR

The southern part of Germany provides a mixture of all soil macropore classes. Soils with ‘no macropore flow’ mainly occur in the river valley areas (e.g. in the Rhine Rift), whereat soils with ‘moderate’ and ‘high macropore flow’ are often found on top of the Mesozoic rock base (e.g. in central and eastern Baden-Württemberg). The close-up view of northern Rhineland-Palatinate in

Figure 17 shows a well-defined area of soils that feature ‘no macropore flow’, which is surrounded by soils that feature ‘moderate’ or ‘high macropore flow’. In this area, Pleistocene pumice stone, ashes and tuff of the Eifel-region with a high hydraulic conductivity are classified in contrast to the surrounding low permeable soils that originate from lower Devonian sediments such as claystone, sandstone or shales. The southern part of Bavaria is mainly divided by the geological units of the upper Pleistocene with its highly permeable sediments of gravel and sand and the deposits of the upper Freshwater Molasse from the Miocene. The Pleistocene sediments are mostly located in the river valleys and in southern Bavaria. Due to their high hydraulic conductivity, ‘no macropore flow’ is assumed at these locations. The sediments of the Miocene scatter from gravel and sand to clayey and marly sediments with lower hydraulic conductivity. They are therefore mainly classified as soils with ‘moderate macropore flow’ but sometimes as soils with ‘high macropore flow’.

4.3.3 Technical concepts to consider preferential flow in PELMO

Three concepts have been discussed during the project how preferential flow can be technically considered in PELMO. The existing macropore flow module considering a fast water transport from the soil surface into the subsoil according to Klein (2012, 2020), the reduction of the field capacity in different soil layers, and the increase of the dispersion length in the whole soil profile are simple approaches to potentially fulfil this requirement. They are explained and compared in the following sections.

4.3.3.1 The static and dynamic macropore module in PELMO

It is already described for PELMO (Klein, 2012, p. 38) that “the concentration of pesticides entering macropores at the soil surface is calculated using the mixing depth concept, whereby incoming rainfall is assumed to mix perfectly with the resident water in a shallow surface layer of soil according to the following equation:

$$Q_1\left(\frac{z_d}{\Delta z}\right) = c_{ma}\left(R + z_d\left(\theta_{mi} + \rho\, k_f\, c_{ma}^{\frac{1}{n}-1}\right)\right) \tag{1}$$

c_{ma}: concentration in the macropore (g cm^{-3})

Δz: thickness of the top numerical layer (cm)

z_d: mixing depth (cm)

Q_1: amount of pesticide stored in the top numerical layer at the previous time step (g cm^{-2})

R: rainfall amount during the time step (cm)

θ_{mi} soil matrix water content (cm^3 cm^{-3})

ρ : the bulk density (g cm^{-3})

$1/n$: Freundlich exponent (-)

k_f: Freundlich sorption coefficient (cm^3 g^{-1})“

“The flux of pesticide into the macropores is given by c_{ma} multiplied by the infiltration rate into macropores Ima, and this amount of pesticide is extracted from the concentration in the matrix to maintain the mass balance.

$$J_{mar} = c_{ma} I_{ma} \tag{2}$$

c_{ma}: concentration in the macropore (g/cm³)

I_{ma}: Amount of water routed into macropore (cm)

J_{ma}: Flux of pesticide into the macropore (g/cm²)" (Klein, 2012, p. 39)

A fixed depth in the soil profile is defined for the length of the macropore for all soil profiles. The amount of water routed through macropores is calculated based on a threshold model. If the rainfall remains below the threshold of 10 mm/d no macropore flow will be considered on this day. If the daily rainfall is above 10 mm the amount of water routed through macropores is calculated as described in the equation below. Depending on the amount of water routed into macropores, a defined proportion of the chemical substance is directly transported in one day from the soil surface, where the macropore is filled with water and substance, until the end of the macropore, where water and substance is released into the soil matrix system. At this defined soil depth percolate is distributed in the soil matrix system independent of the actual soil moisture conditions. In the soil layers between the soil surface and the end of the macropore, there is no exchange of percolate between the macropore domain and the soil matrix domain. The existing version of the macropore module in PELMO follows a static system, which means that the percolate flow in the macropore domain constantly depends on the amount of daily precipitation and does not consider different seasonal soil moisture contents for the efficacy of the macropore domain.

$$\begin{aligned} &I_{ma} = 0, \quad I_{mi} = R \quad \text{if} \quad R \le I_c \\ &I_{ma} = f(R - I_c), \quad I_{mi} = (1-f)(R - I_c) + I_c \quad \text{if} \quad R > I_c \end{aligned} \tag{3}$$

I_{ma}: amount of water routed into macropore (cm)

I_{mi}: amount of water routed into soil matrix (cm)

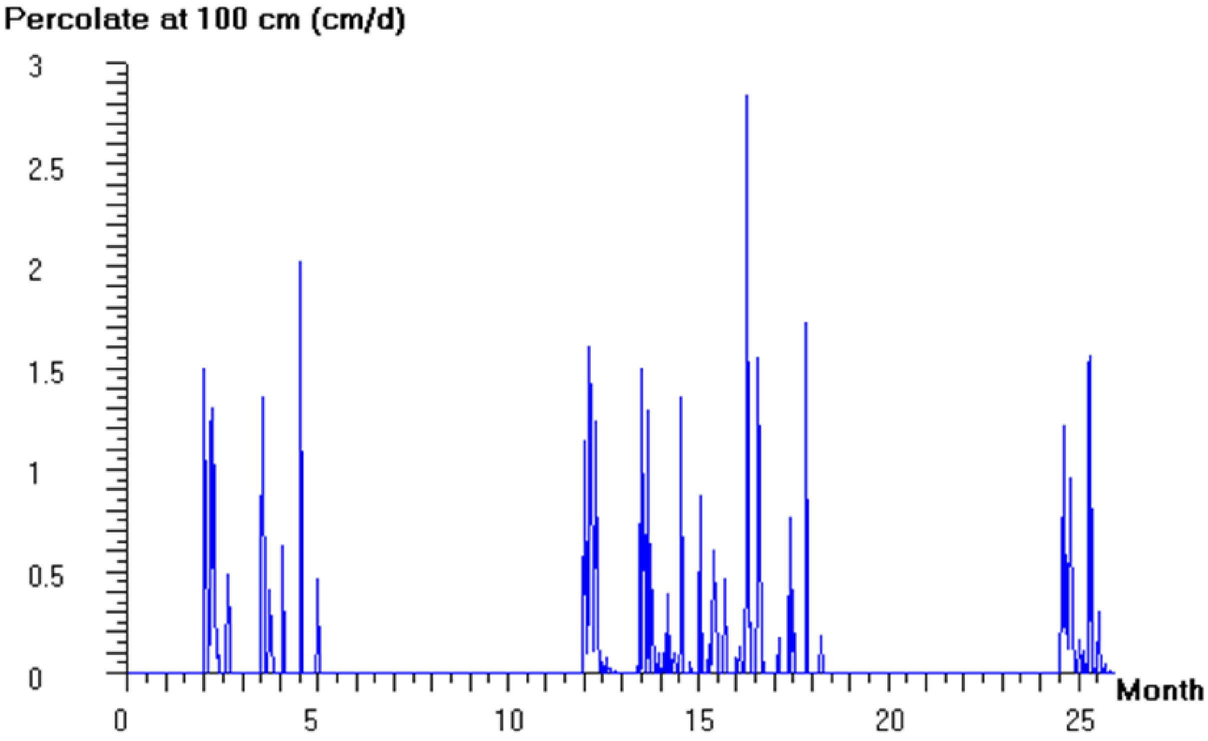
I_C: threshold daily rainfall which generates infiltration into macropores (cm)

R: daily rainfall (cm)

f: fraction of the excess rainfall which is routed into macropores (-)

In the current project, the existing static macropore flow module in PELMO was extended to a dynamic macropore flow module, which additionally considers soil moisture contents to define the intensity of preferential flow in the macropore domain of the soil profile over time. The idea behind is to account for drying-out soils during longer periods without rainfall. The fraction of percolate water during intensive rain, which flows into the macropore domain depends on the soil moisture conditions during the last 7 days before the intensive daily rain event. For this analysis, the soil moisture content in the soil profile is calculated and recorded in PELMO over the total length of the macropore (e.g. 80 cm). If the soil, for example, was wet during the last 7 days the fraction of rainwater, which enters the macropore domain (f) would be set to a defined minimum fraction (or could be zero) and minimal (or no) preferential flow occurs during modelling. This approach refers to bio-pores, which can be available independent on actual soil moisture conditions. If the maximum soil water deficit in the soil column was above 50 % (at least at one of the 7 days) the maximum fraction of rainwater entering the macropore domain (f) is used. It is assumed that in such a situation a higher number of shrinkage cracks could be formed. Between both boundary conditions of the soil moisture content, the fraction of rainwater entering the macropore domain (f) is linearly interpolated. Independent of the dynamic or static approach, the macropore flow module has a very limited influence on the total amount of percolate amount reaching the 1 m soil depth as demonstrated in Figure 18 and Figure 19.

Figure 18: **PELMO Screenshot: Daily percolate amounts calculated with FOCUS PELMO (FOCUS Hamburg scenario, winter cereals, FOCUS parametrisation with chromatographic flow only)**

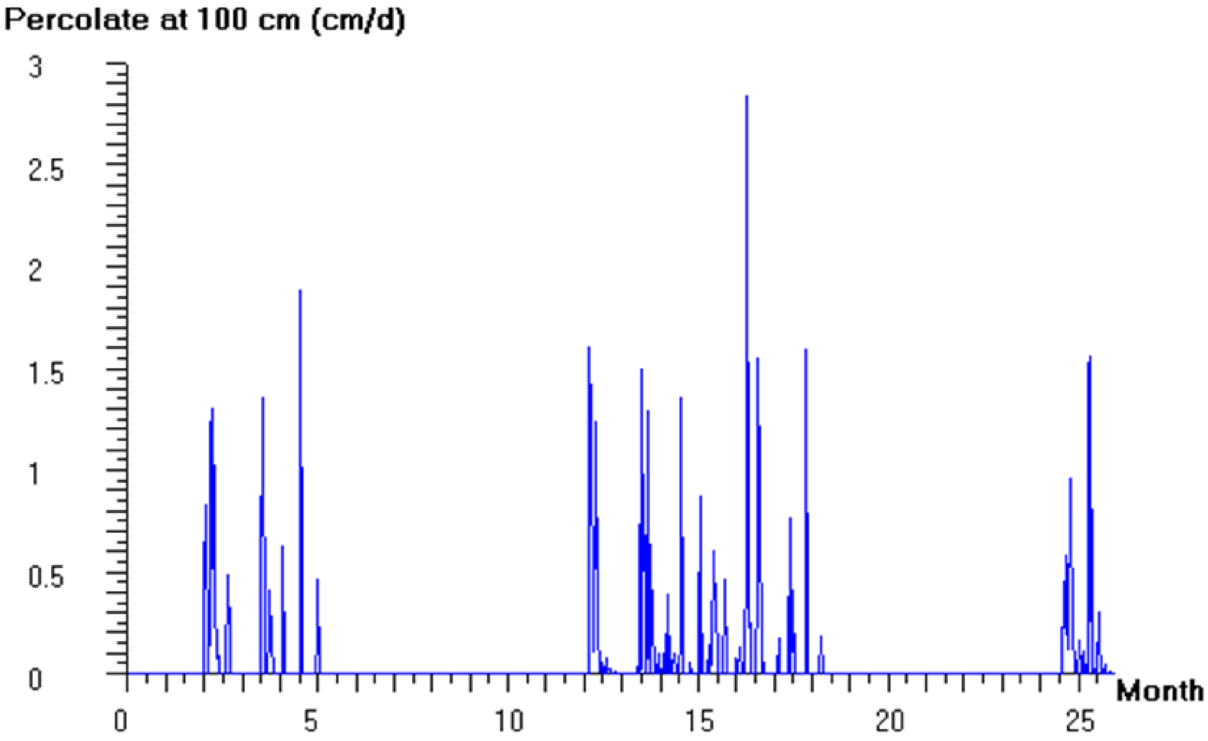


Source: own illustration, Fraunhofer IME

For the simulation shown in Figure 19 a static fraction of 10 % preferential flow of daily precipitations was defined. A threshold of 10 mm rain per day was implemented to generate preferential flow. Lower daily precipitation amounts do not lead to an activation of preferential flow in PELMO. The macropore system was defined between 0 and 80 cm soil depth.

Figure 19: PELMO screenshot: Daily percolate amounts calculated with FOCUS PELMO (FOCUS Hamburg scenario, winter cereals, FOCUS parametrisation with chromatographic flow plus macropore module)

For the simulation a static fraction of 10 % preferential flow of daily precipitations was defined. A threshold of 10 mm rain per day was implemented to generate preferential flow. Lower daily precipitation amounts do not lead to an activation of preferential flow in PELMO. The macropore system was defined between 0 and 80 cm soil depth.



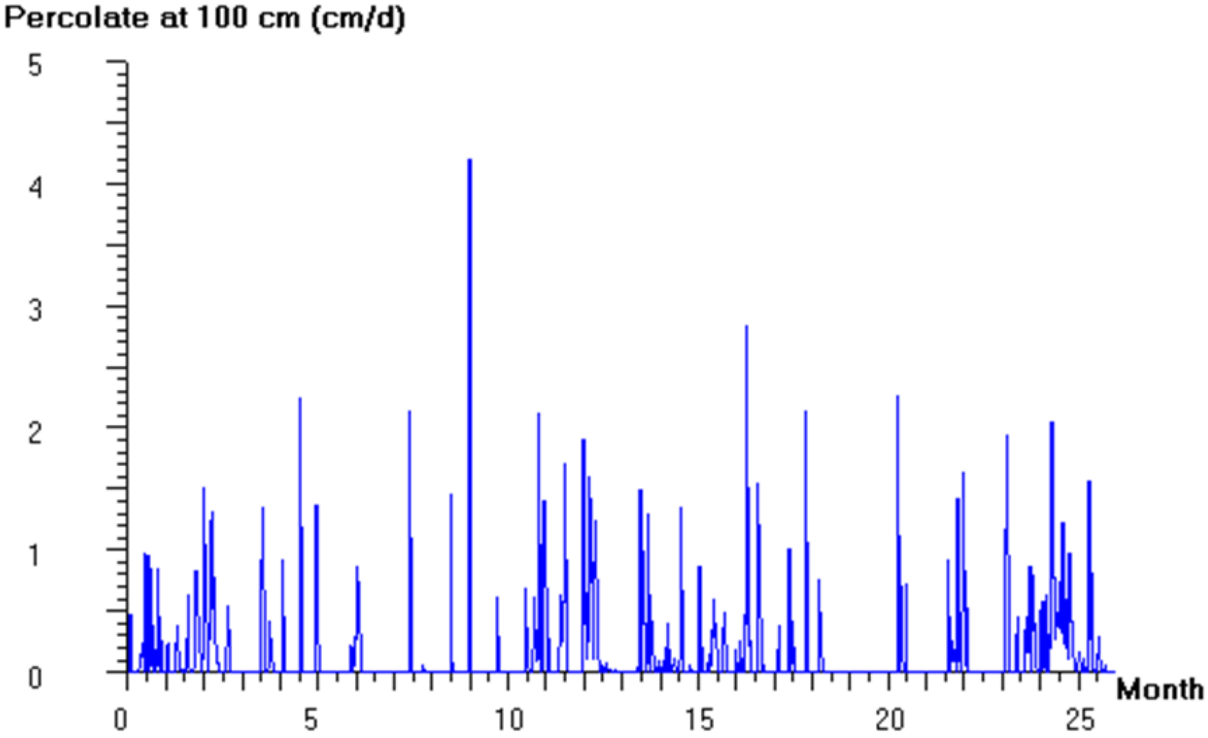
Source: own illustration, Fraunhofer IME

4.3.3.2 Reduction of field capacity

The soil moisture in PELMO is calculated based on the capacity approach: The transport of water through the soil is basically driven by the difference of field capacity and wilting point (i.e., the available soil moisture) in the different soil layers. However, the available soil moisture itself is not an input parameter in PELMO, but it is internally calculated based on field capacity and wilting point. The transport of water fluxes to deeper soil layers is initiated as soon as the soil moisture content achieves the field capacity and stops again when the soil moisture content falls below the field capacity.

A reduction of the field capacity in PELMO will induce an earlier and stronger transport of water to deeper soil layers during rain events. Consequently, pesticides will be transported through the soil column to a higher extend compared to the original parametrisation. This approach of soil scenario adjustment was already used for the parametrisation of the PELMO railway scenarios, which are characterised by a high content of gravel and rocks. By reducing the field capacity, the water movement in these scenarios was significantly increased (Klein 2002). Figure 20 shows the effect of the reduction of field capacity to 25 % on the daily percolate amounts calculated with PELMO for the same situations as before: Significantly higher amounts of percolate are simulated compared to the previous examples in Figure 18 and Figure 19.

Figure 20: PELMO screenshot: Daily percolate amounts calculated with FOCUS PELMO (FOCUS Hamburg scenario, winter cereals, FOCUS parametrisation with chromatographic with 25 % reduced field capacity)



Source: own illustration, Fraunhofer IME

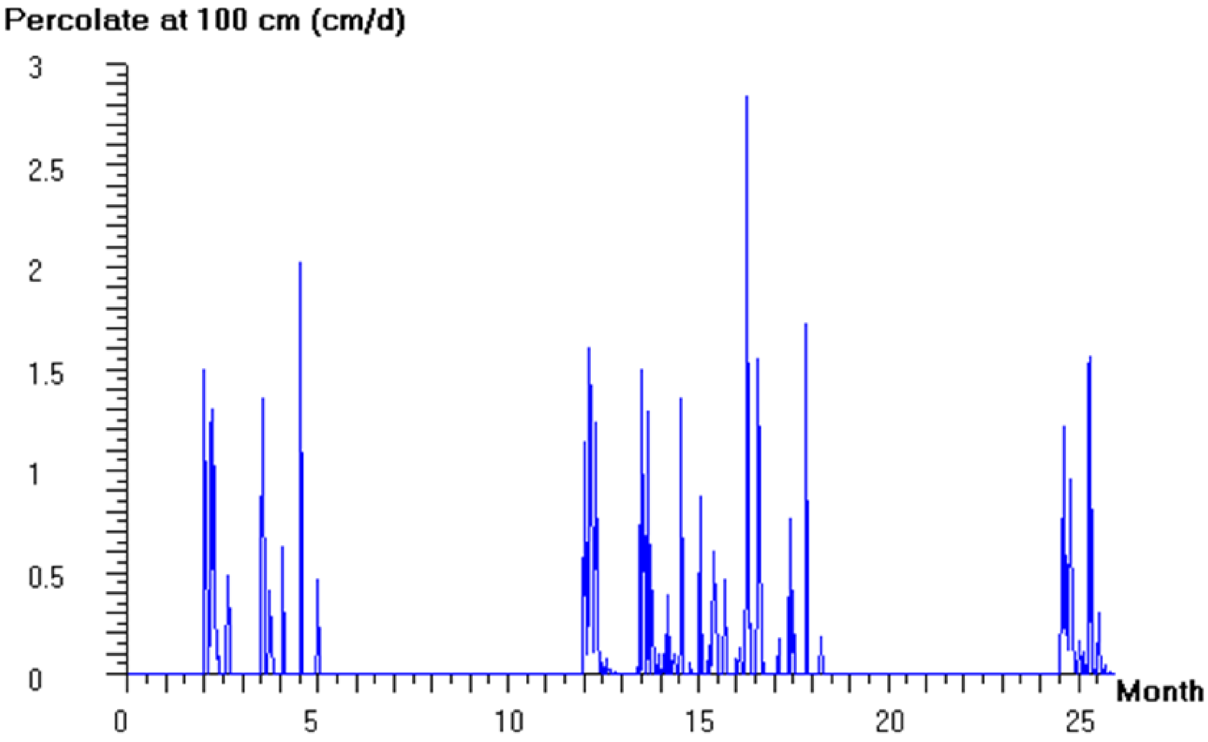
4.3.3.3 Increase of dispersion length

According to the harmonisation of the FOCUS scenarios and FOCUS models, the dispersion length in FOCUS PELMO was increased from 2.5 cm (FOCUS 2000) to 5 cm (European Commission 2014).

This adjustment did not lead to any change of the soil moisture content in the FOCUS soil scenarios and the resulting percolate amounts, but it had a major impact on the percolate concentrations at 1 m soil depth as shown by a comparison presented in European Commission (2014).

An increase of the soil dispersion length leads to a widening of the vertical concentrations profile of a chemical substance, which basically means that a certain portion of the substance is transported faster to deeper soil layers. Nevertheless, the core area of the concentration bulk (the maximum peak) in soil at a given time is not affected. Therefore, the faster transport of portions of the substance leads to an earlier breakthrough at 1 m soil depth. The main difference of this approach compared to the reduction of the soil moisture content is that the total water transport in the soil profile over time is not changed. Higher substance concentrations in percolate are calculated without a massive change of the soil hydrology. An example of percolate amounts calculated wit PELMO with an increased dispersion length by a factor of four is provided in Figure 21 and shows the same pattern for the daily percolate amounts as Figure 18 where the FOCUS standard modelling routine was used.

Figure 21: PELMO screenshot: Daily percolate amount calculated with FOCUS PELMO (FOCUS Hamburg scenario, winter cereals, increased dispersion length)



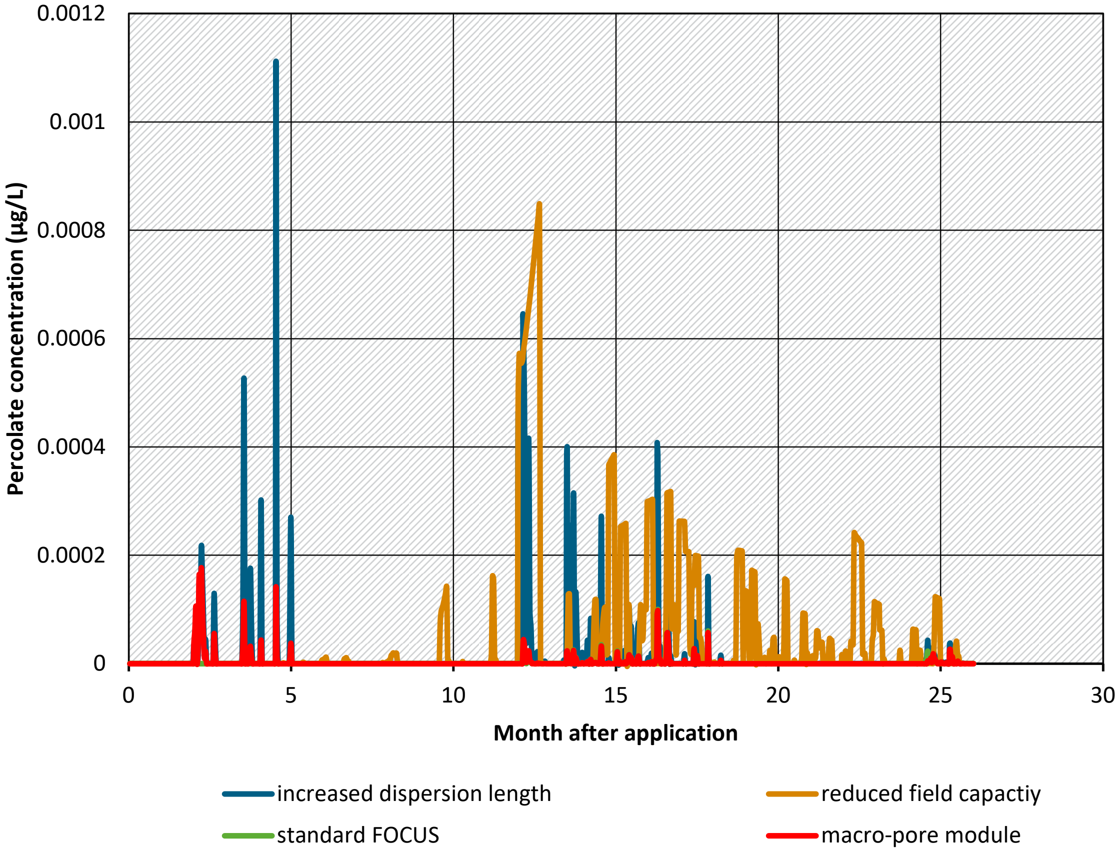
Source: own illustration, Fraunhofer IME

4.3.3.4 Comparison of the three technical concepts to consider preferential flow in PELMO

Calculated percolate concentrations of an active substance in 1 m soil depth of the FOCUS Hamburg scenario are presented in Figure 22 to illustrate the impact of the three different technical options in PELMO to adjust the standard model assumptions to preferential flow. All calculations are based on standard parametrisation in FOCUS PELMO, which are suggested by European Commission (2014). For the simulations an artificial active substance (FOCUS Dummy D) with a $DegT_{50}$ of 20 days and a K_{foc} of 60L/kg was used in combination with a single application of 1 kg/ha in winter cereals one day before crop emergence. Compared to the FOCUS standard (Standard, Figure 18), field capacity was reduced about 25 % (25 % FK) and dispersion length was increased by a factor of 4 up to 20 cm (DISP 20 cm). For the simulation run with the static macropore module (macropore flow) a fraction of 10 % of daily precipitations was defined which enters the macropore domain. A threshold of 10 mm rain per day was used to generate preferential flow. Lower precipitation amounts do not lead to an activation of preferential flow. The macropore domain was defined between 0 and 80 cm soil depth.

The results in Figure 22 demonstrate that principally all three technical options in PELMO can be used to simulate an earlier breakthrough of the active substance FOCUS Dummy D in the percolate compared to the original FOCUS standard parametrisation in PELMO. The green line near zero demonstrates basically no appearance of the active substance in the first 30 months after application, when the FOCUS standard modelling routine is used. In contrast, based on the two technical approaches ´macropore module´ and ´increased dispersions length´, first evidence of the active substance in the percolate is calculated already two months after application. The third option of a ´reduced field capacity´ (orange line in Figure 22) leads to a similar pesticide transport, but with a significantly delayed breakthrough of the active substance in 1 m soil depth.

Figure 22: **Comparison of calculated percolate concentration for four simulation runs with different technical adjustments in PELMO after a single application of 1 kg/ha one day before crop emergence in winter cereals (FOCUS Hamburg, example compound FOCUS D with DegT$_{50}$: 20 d, K$_{foc}$: 60 L/kg)**



Source: own illustration, Fraunhofer IME.

4.3.4 Calibration of preferential flow in PELMO

The previously discussed options to consider preferential flow in PELMO were never tested in terms of their impact on modelling results and the prediction of leachate concentrations compared to measured data in different soils. Therefore, the objective in this section is to analyse whether the preferential flow options in PELMO provide comparable results to experimental data, at least on an intended aggregated level regarding average annual pesticide concentrations. It must be considered that the quality and quantity of available targeted experimental data are limited to calibrate leaching models like PELMO. The following experimental data were selected and made available for a comparison with different technical modelling routines in PELMO: monitoring data from the Danish Pesticide Leaching Assessment Programme (PLAP) and measured data from lysimeter studies.

In addition, a comparison of PELMO results by using preferential flow routines with the results of model MACRO (Larsbo & Jarvis 2003) is performed. The model MACRO was developed in Sweden for soils affected by preferential flow and recommended already by the first FOCUS groundwater group as a suitable tool to estimate leaching for those kinds of soils. For that purpose, a preferential flow scenario for the FOCUS location Châteaudun was developed (FOCUS 2000).

In contrast to the capacity model PELMO the model MACRO is a deterministic model which explicitly solves the Richard’s equation. A complete water balance is considered in the model including unsaturated and saturated water flow, canopy interception and root water uptake. MACRO can be used to simulate non-reactive tracers (e.g. bromide, chloride) or pesticides and includes descriptions of processes such as convective-dispersive transport, canopy interception and wash-off, sorption, biodegradation and plant uptake. The model may be run in either one or two flow domains with no change in the hydraulic properties assumed to characterise the soil scenario. This allows a quantitative evaluation of the impact of macropore flow on solute transport processes. In two domains, macropores and micropores operate separately, though interacting, flow regions, each characterized by a degree of saturation, conductivity and a flux. In case macropores are not considered for a simulation the model uses the standard Richards' and convection-dispersion equations (similar as PEARL). Sensitive input parameters for MACRO and for PELMO are the daily precipitation, the organic carbon content in soil as well as the degradation half-life ($DegT_{50}$) and the sorption constant (K_{foc}) of the chemical compound. Additionally, all macropore parameters are very sensitive to leaching (e.g. the mass transfer coefficient between the two soil domains and the fraction of sorption sites in the macropore domain). A calibration of those model assumptions is difficult since these parameters cannot be directly measured.

In the following section it is evaluated how far PELMO simulations using the macropore flow module or increased dispersion length are able to predict a similar leaching behaviour as measured in loamy soils from the above-mentioned Danish Pesticide Leaching Assessment Programme (PLAP).

4.3.4.1 PLAP monitoring data and model parametrisation

Targeted pesticide monitoring data from the Danish Pesticide Leaching Assessment Programme (PLAP) are annually reported (e.g. Brüsch et al. 2016, Rosenbom et al. 2021). Five and currently six monitoring sites with different soil and climate conditions representative for Denmark are included in the monitoring strategy of PLAP (Lindhardt et al. 2001, Haarder et al. 2021). The sites Tylstrup and Jyndevad represent sandy soil conditions, and the sites Silstrup, Estrup and Faardrup represent rather loamy soils with higher clay contents. The leaching behaviour of specific active substances like metribuzin, azoxystrobin, glyphosate and fluazifop-P-butyl and their metabolites on those Danish fields are evaluated in Kjær et al. (2005), Jørgensen et al. (2012), Norgard et al. (2014, 2015) and Vendelboe et al. (2016). An overall long-term evaluation of PLAP results is provided in Rosenbom et al. (2015), and rapid preferential transport through well-connected discontinuities such as wormholes and fractures was identified to enable the pesticides to bypass the otherwise retarding plough layer at the loamy soil sites. In another project, the PLAP monitoring data from about 50 active substances and 50 degradation products was compared to predicted environmental concentration in groundwater (PECgw) obtained using the regulatory models FOCUS PELMO (Hamburg scenario) and FOCUS MACRO (Karup and Langvad scenarios) (Pullan et al. 2016). For the analysis of PLAP data with PELMO, long term climate data and substance concentrations in the drainage systems for the different time periods from three PLAP fields were made available by the Geological Survey of Denmark and Greenland (GEUS) and the University of Aarhus (see frame below). An overview about the soil properties of the PLAP fields Silstrup, Estrup and Tylstrup is given in Table 15, Table 16 and Table 17, respectively.

Monitoring data from Danish Pesticide Leaching Assessment Programme (PLAP)

The following targeted monitoring data from Danish Pesticide Leaching Assessment Programme (PLAP) were provided from the Geological Survey of Denmark and Greenland (GEUS) and the University of Aarhus for the calibration of preferential flow in PELMO:

Estrup:

September 2000 - January 2013
The concentration of glyphosate and AMPA [µg L^{-1}] in samples was collected from sub-samples proportional to the tile drainage

May 2004 to June 2009
The concentration of azoxystrobin and R234886 [µg L^{-1}] in samples was collected from sub-samples proportional to the tile drainage.

Silstrup

July 2008 - June 2013
The concentration of fluazifop-P-butyl and TFMP [µg L^{-1}] in samples was collected from groundwater.

May 2004 to July 2010
The concentration of azoxystrobin and R234886 [µg L^{-1}] in samples was collected from sub-samples proportional to the tile drainage.

Tylstrup

September 1999 – June 2003.
The concentration of the two metribuzin degradation products diketo-metribuzin (DK) and -desaminodiketometribuzin (DADK) [µg L^{-1}] in samples was monthly collected from suction cups in 1 m and 2 m depth and from groundwater.

Table 15: Properties of the Silstrup^ soil profile used in PELMO

Horizon	Depth [cm]	Sand [%]	Clay [%]	FC [cm³/cm³]	WP [cm³/cm³]	OC [%]	Density [kg/L]	Biodeg. Factor [-]
Ap	0-30	62.0	18.3	0.345	0.135	1.80	1.50	1.0
B1	30-50	55.3	30.1	0.325	0.135	0.29	1.50	0.5
B2	50-80	55.3	30.1	0.325	0.135	0.20	1.50	0.3

^ Macropore class: high macropore flow (> 25 % clay), FC: field capacity, WP: wilting point, OC: organic carbon content

Table 16: Properties of the Estrup^ soil profile used in PELMO

Horizon	Depth [cm]	Sand [%]	Clay [%]	FC [cm³/cm³]	WP [cm³/cm³]	OC [%]	Density [kg/L]	Biodeg. Factor [-]
Ap	0-25	70.8	13.8	0.310	0.090	1.57	1.60	1.0
Ap2	25-30	47.8	36.3	0.310	0.090	0.93	1.60	1.0
BEv	30-45	47.8	36.3	0.300	0.200	0.29	1.73	0.5
BEv	45-50	50.9	33.0	0.300	0.200	0.12	1.73	0.5
Bv	50-80	50.9	33.0	0.300	0.200	0.20	1.73	0.3
Bv	80-100	50.9	33.0	0.300	0.200	0.00	1.73	0.3

^ Macropore class: high macropore flow (> 25 % clay), FC: field capacity, WP: wilting point, OC: organic carbon content

Table 17: Properties of the Tylstrup* soil profile used in PELMO

Horizon	Depth [cm]	Sand [%]	Clay [%]	FC [cm³/cm³]	WP [cm³/cm³]	OC [%]	Density [kg/L]	Biodeg. Factor [-]
Ap	0-25	70.8	13.8	0.310	0.090	1.57	1.60	1.0
Ap2	25-30	47.8	36.3	0.310	0.090	0.93	1.60	1.0
BEv	30-45	47.8	36.3	0.300	0.200	0.29	1.73	0.5
BEv	45-50	50.9	33.0	0.300	0.200	0.12	1.73	0.5
Bv	50-80	50.9	33.0	0.300	0.200	0.20	1.73	0.3

* Macropore class: no macropore flow (sandy soil), FC: field capacity, WP: wilting point, OC: organic carbon content

In addition to the basic soil information other parameters must be defined for the macropore flow module in PELMO (Table 18). The threshold of precipitation amount that induces macropore flow from the soil surface was set to 10 mm in 24 hours to ensure that only heavy rainfall events will lead to fast preferential transport. The depth of the macropore end was fixed in all sites or scenarios to 80 cm in the soil profile. A dynamic modelling of preferential flow depending on the soil moisture content over time was used. The parameters that were modified differently in the dynamic approach are the minimum and maximum fraction of macropore flow in relation to the total flow as shown in the following table. Additional simulations were performed with an increased dispersion length of 10 cm (='DISP10'). The standard PELMO simulations based on chromatographic flow with a dispersion length of 5 cm was also performed (='standard').

Four active substances from plant protection products were applied at Silstrup, Estrup and Tylstrup during the period when weather data were available: Silstrup with high precipitation between 2003-2014, Estrup with rather low precipitation between 2000-2013 and Tylstrup with high precipitation between 1999-2003. Available information about pesticide applications at the three PLAP sites is provided in Table 19. Table 20 shows key pesticide properties used for the PELMO simulations. Plant uptake was not considered in the simulation runs.

Table 18: Additional parameters defined in PELMO to simulate preferential flow

Variations of dynamic macropore flow simulations (minimum and maximum fraction) together with a simulation considering an increased dispersion length of 10 cm (DISP10)

Parameter	2% to 5%	4% to 8%	5% to 10%	5% to 15%	DISP10
Dispersion length (cm)	5	5	5	5	10
Depth end of macropores (cm)	80	80	80	80	-
Min. fraction of macropore flow in relation to total flow (-)	0.02	0.04	0.05	0.05	-
Max. fraction of macropore flow in relation to total flow (-)	0.05	0.08	0.10	0.15	-
Threshold rainfall that induces macropore flow from soil surface (mm/24h)	10	10	10	10	-
Dynamic moisture dependency for macropore flow (yes/no)	yes	yes	yes	yes	no

Table 19: Active substance application at three PLAP sites

Substance	Field	Crop during application	Application date	Application rate [g/ha]	Interception [%]
Azoxystrobin	Estrup	spring cereals	22/06/2004	250	90
Azoxystrobin	Estrup	spring cereals	29/06/2006	250	90
Azoxystrobin	Estrup	winter cereals	13/06/2008	250	90
Azoxystrobin	Estrup	spring cereals	04/06/2009	250	90
Azoxystrobin	Estrup	spring cereals	13/06/2012	250	90
Azoxystrobin	Estrup	winter cereals	02/06/2014	250	90
Azoxystrobin	Silstrup	spring cereals	14/06/2004	250	90
Azoxystrobin	Silstrup	spring cereals	30/06/2005	250	90
Azoxystrobin	Silstrup	winter cereals	24/06/2009	250	90
Glyphosate	Estrup	bare soil	13/10/2000	1440	0
Glyphosate	Estrup	bare soil	02/09/2002	1440	0
Glyphosate	Estrup	bare soil	09/09/2005	1440	0
Glyphosate	Estrup	bare soil	24/09/2007	1020	0
Glyphosate	Estrup	bare soil	03/10/2011	1360	0
Glyphosate	Estrup	bare soil	21/08/2013	1080	0
Fluazifop-P-butyl	Silstrup	Sugar beet	01/07/2008	375	20
Fluazifop-P-butyl	Silstrup	Grass	02/05/2010	188	90

Substance	Field	Crop during application	Application date	Application rate [g/ha]	Interception [%]
Fluazifop-P-butyl	Silstrup	Grass	26/04/2011	188	90
Fluazifop-P-butyl	Silstrup	Grass	19/04/2012	188	90
Metribuzin	Tylstrup	Potatoes	25/05/1999	140	0
Metribuzin	Tylstrup	Potatoes	07/06/1999	105	0

* Standard parameters for fate on canopy considered (wash-off and lumped disappearance)

Table 20: Pesticide properties considered in the simulation runs with PELMO

The degradation of metabolite CyPM in soil was evaluated as pH dependent during EU assessment. A geometric mean DT50 of all soils of 55.4 d represents a pH value of 7.3 according to the linear regression line and was considered in the project as appropriate input parameter for modelling for the measured pH ranges at the Estrup and Silstrup fields (see *).
The adsorption of metabolite CyPM in soil was evaluated as pH dependent during EU assessment. The geometric mean K$_{foc}$ of all soils of 83 and the arithmetic mean 1/n value of 0.80 represent a pH value of 6.5 or 7.3 depending on the mathematic correlation used and were considered in the project as appropriate input parameter for modelling for the measured pH ranges at the Estrup and Silstrup fields (see **).
The formation of DADK by DA via photolysis was not considered since soil photolysis can only be considered for the active substance (see ***)

Substance	Molecular mass [g/mol]	Formation fraction [-]	DegT$_{50}$ [d]	K$_{foc}$ [L/kg]	Freundlich [-]
Azoxystrobin	403.4	-	78.0	423	0.86
CyPM	398.4	0.874	55.4*	83**	0.80**
Glyphosat	169.1		20.5	15388	0.93
AMPA	111.0	0.36	88.8	9749	0.81
Fluazifop-P-butyl	383.4	-	0.3	3394	1.0
FP	327.4	1.0	9.1	48.7	0.90
TFMP	163.0	0.4	75.3	24.7	0.84
Metribuzin	214.3	-	7.1	49.7	0.87
U1	168.2	0.29 (from metribuzin)	0.2	13.7	0.99
DK	184.2	0.24 (from metribuzin)		DK	184.2
DA	199.3	0.16 (from metribuzin)	10.3	43.7	0.92
DADK	169.2	0.48 (from DA)0.82 (from DK)***	9.1	29.3	0.94

Table 21 shows some information about the climate during the simulation. Most sensitive weather data (precipitation) were taken from measured data at the PLAP sites. Other weather parameters needed for PELMO (e.g. temperature, potential evapotranspiration) were derived from the MARS database considering weather stations close to the monitoring sites. An overview is given in the following table. The weather data from the MARS database was used to perform long-term simulations over 26 years in a similar way as standard FOCUS simulations. Unfortunately, a comparison of rainfall data between MARS and PLAP showed significant differences between both sources. To derive comparable rainfall data, the daily precipitation data from MARS was scaled to measured weather data from PLAP fields based on the overlapping period. A similar scaling procedure has been performed also for some of the FOCUS scenarios (FOCUS 2000).

Table 21: Climate data considered in the simulations with PELMO

The scaling factor was used only during the overlapping period, when both site-specific weather data and MARS weather data were available (see *)

Parameter	Estrup	Silstrup	Tylstrup
Altitude (m)	49	4	19
Longitude (°)	9.048	8.64	9.95
Latitude (°)	55.485	56.88	57.12
PLAP period (-)	2000-2013	2003-2014	1999-2003
Annual average precipitation PLAP (mm /a)	1107	967	986
MARS cell no (-)	122107	128106	129109
Longitude (MARS, °)	9.07	8.62	9.87
Latitude (MARS, °)	55.53	57.12	56.88
MARS period (-)	1990-2016	1990-2016	1990-2016
Annual average precipitation MARS (mm /a)*	778	725	656
Scaling factor* (-)	1.423	1.334	1.503

4.3.4.2 Comparison of measured and modelled PLAP results

Only the results for azoxystrobin and its metabolite CyPM are finally presented in this section because they were applied at two PLAP sites (Estrup and Silstrup). The results for the other compounds are summarised in Appendix A.

Azoxystrobin and metabolite CyPM at Estrup and Silstrup

According to the soil classification scheme for preferential flow in section 4.3.1 both the Estrup and Silstrup soil profiles belong to class three with a high potential for macropore flow. Therefore, as an initial step for the comparison with measured data from the PLAP monitoring system the same model parametrisations for macropore flow was considered for both sites.

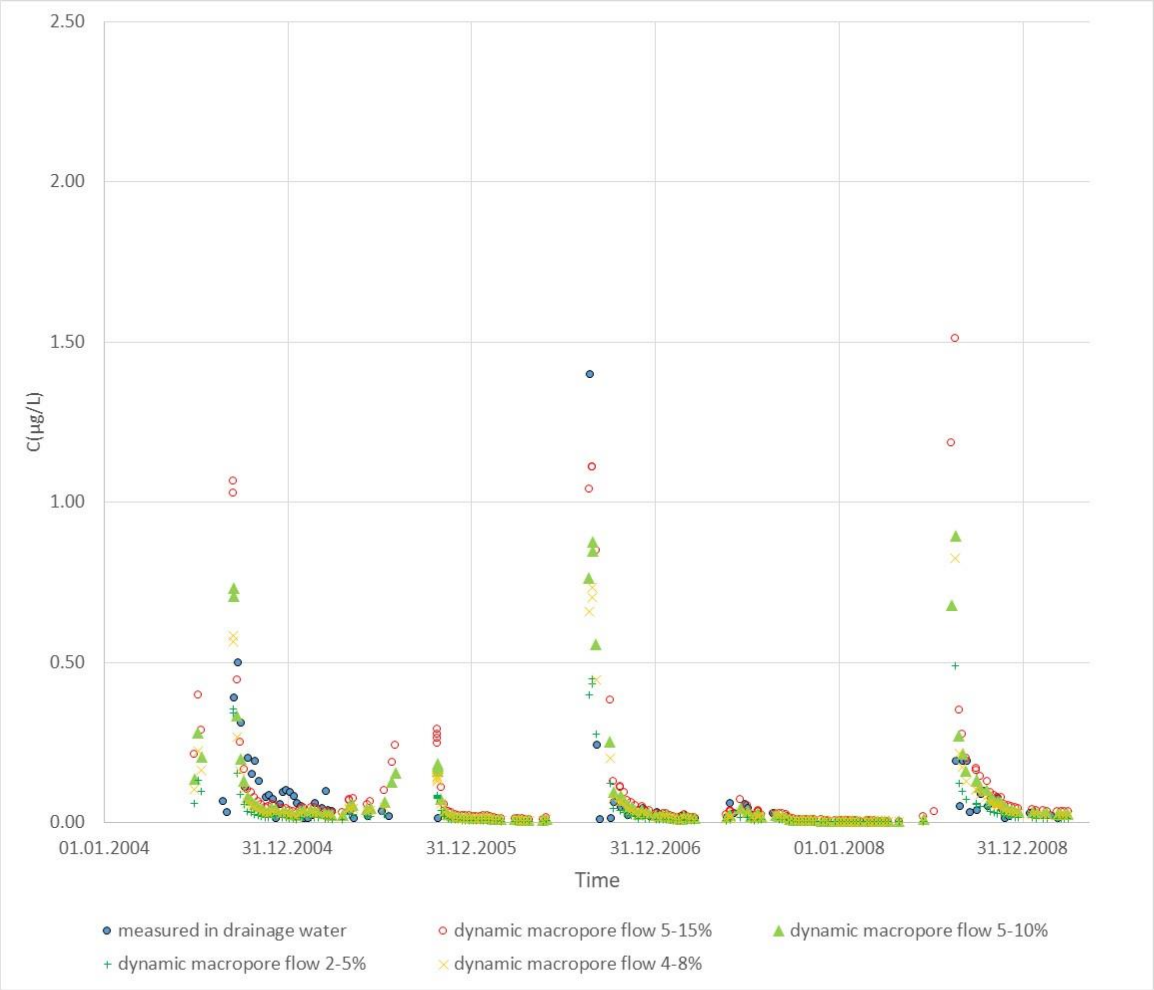
As summarised in Table 19 azoxystrobin was applied six times at Estrup and three times at Silstrup on winter and spring cereals. The nominal application rate was 250 g/ha in all applications at late BBCH stages (EFSA crop interception 90 %). To realistically simulate the fate of the compound the pesticide was applied to the canopy and wash-off was considered in the simulations. It is known that azoxystrobin degrades via soil photolysis. This process was therefore additionally considered in the simulation with PELMO (DT50: 2.6 d at 500 W/m^2). However, during soil photolysis the metabolite CyPM is not formed. Consequently, soil photolysis was considered as an additional sink for the active compound.

Several different simulations were performed with PELMO for both PLAP sites. Because their results are often rather similar, they are not completely presented in one figure. A model run with the FOCUS standard parametrisation, a run with an increased dispersion length of 10 cm and several model-runs using the dynamic macropore module with different minimum and maximum proportions of preferential flow are compared to measured drainage data after leaching in about 1 m soil depth.

For Estrup, the results of several simulations considering the dynamic macropore flow module with different minimum and maximum proportions of the water fluxes used for preferential flow are presented in Figure 23. The simulation based on FOCUS standard parametrisation and the simulation with an increased dispersion length did not lead to any concentrations of azoxystrobin in the percolate and are therefore not presented in Figure 23. The variations with macropore flow show a comparable pattern of leachate concentrations for the active substance as observed in the drainage measurements of the PLAP monitoring.

Figure 23: Measured and modelled azoxystrobin concentrations in the percolate (drainage) at 100 cm at Estrup PLAP site

Different macropore flow variations have been modelled with PELMO. The percentages in the legend refer to minimum and maximum fractions of precipitation used in the dynamic macropore flow model approach.

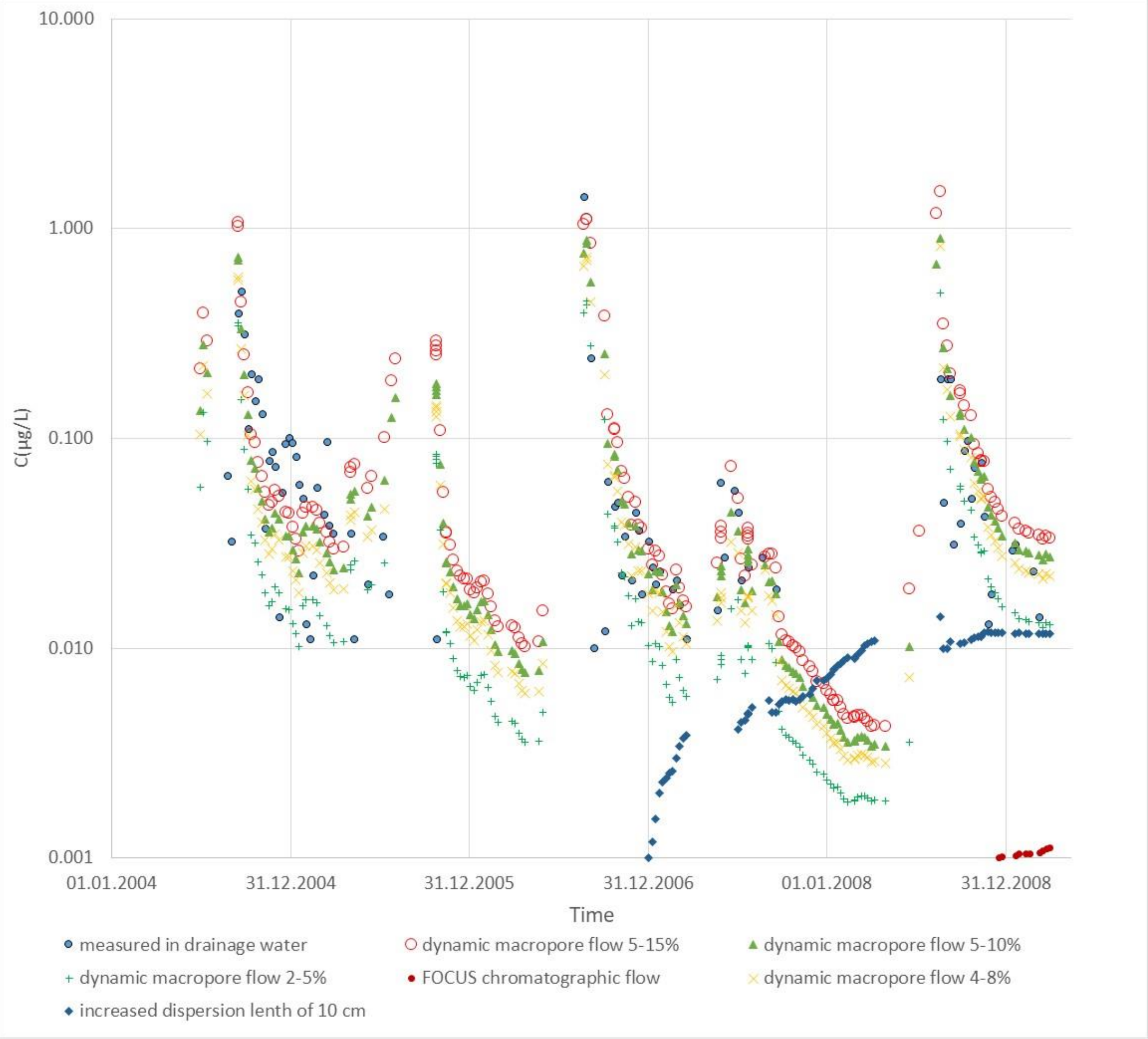


Source: own illustration, Fraunhofer IME.

When using a logarithmic scale in Figure 24 and Figure 25, it becomes obvious that all simulation runs using the dynamic macropore flow module fit best the experimental data showing an early break-through of azoxystrobin after applications. In contrast, the model run with the FOCUS standard parametrisation based on chromatographic flow only and the model run with an increased dispersion length are both not able to cover the experimental data. Deficiencies occur in both simulations considering only chromatographic flow regarding the height and the temporal breakthrough of the active substance concentration in 100 cm soil depth. Without macropore flow, the breakthrough of the active substance at Estrup is modelled about 2.5 years and 4.5 years later than analysed during measurements.

Figure 24: Measured and modelled azoxystrobin concentrations in the percolate (drainage) at 100 cm at Estrup PLAP site with logarithmic scale

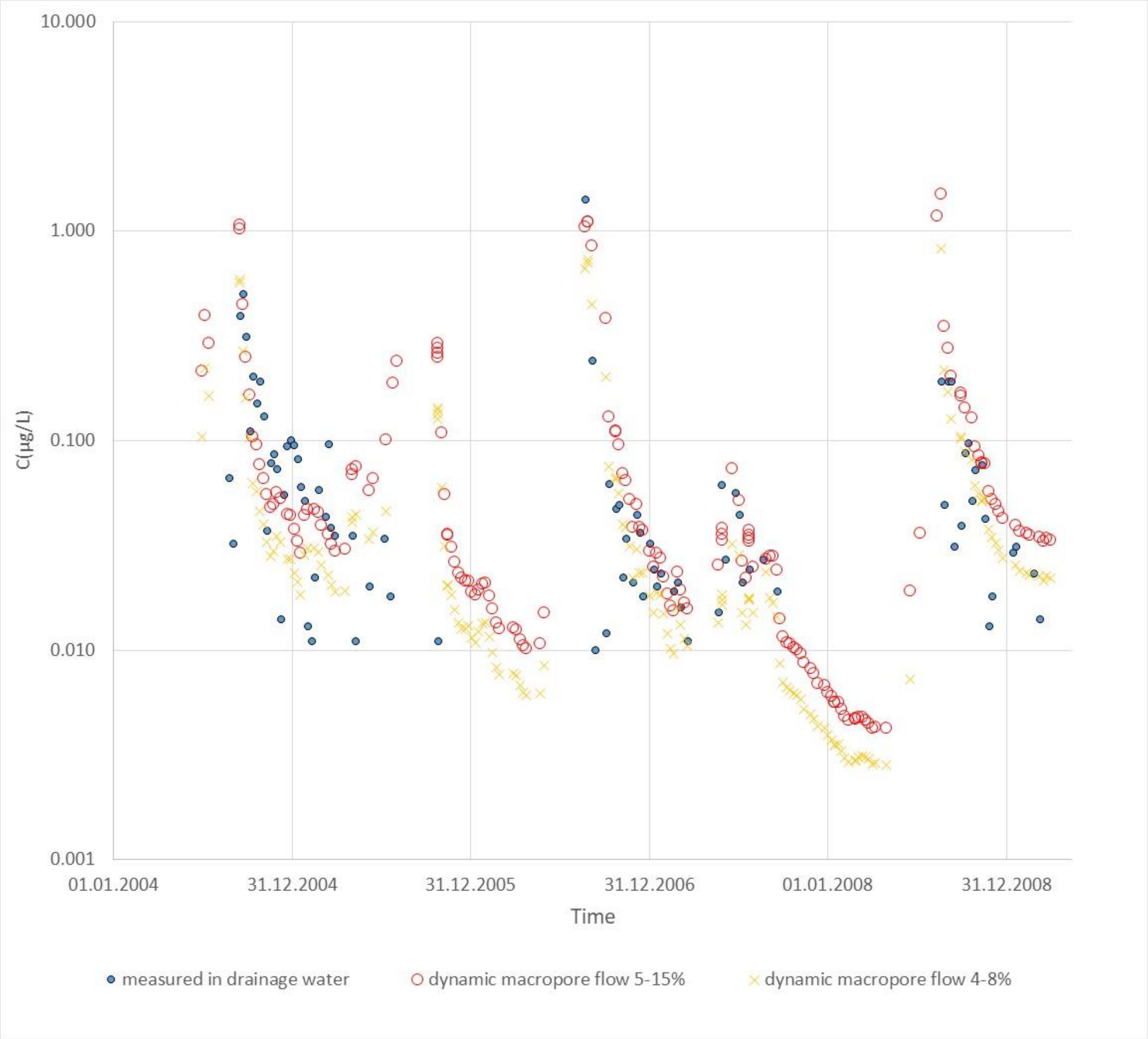
Different dynamic macropore flow variations have been modelled with PELMO and compared to FOCUS standard model parametrisation and an increased dispersion length. The percentages in the legend refer to minimum and maximum fractions of precipitation used in the dynamic macropore flow model approach.



Source: own illustration, Fraunhofer IME.

Figure 25: **Measured and modelled azoxystrobin concentrations in the percolate (drainage) at 100 cm at Estrup PLAP site with logarithmic scale**

Different dynamic macropore flow variations have been modelled with PELMO and compared. The rates in the legend refer to minimum and maximum fractions of precipitation used in two dynamic macropore flow model runs which fit best the experimental data.



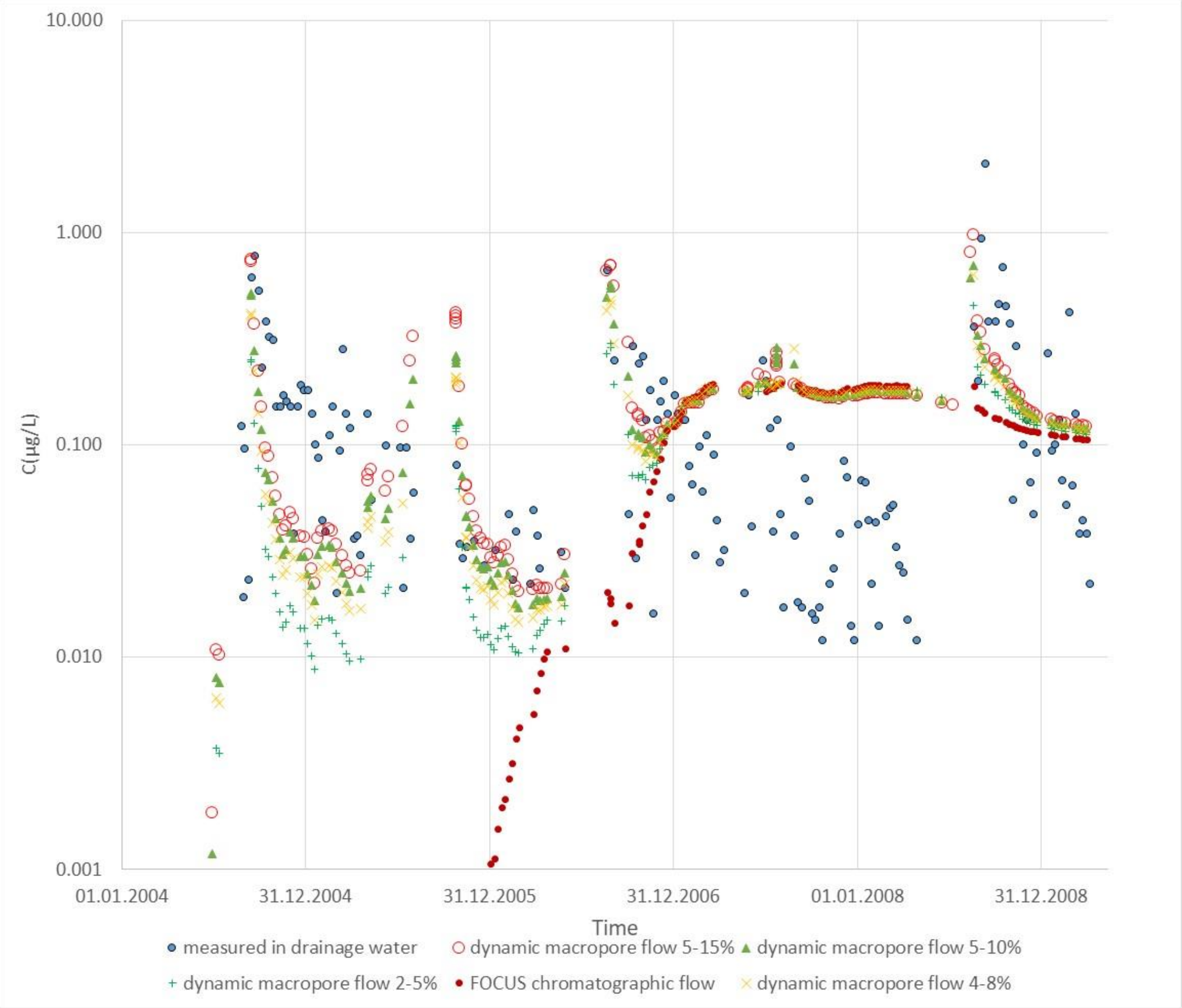
Source: own illustration, Fraunhofer IME

The respective modelling results for the metabolite CyPM from azoxystrobin at Estrup are presented in Figure 26 and Figure 27. Similar as for the active substance the simulation runs based on FOCUS standard parametrisation (chromatographic flow only, dispersion length of 5 cm) and with an increased dispersion length of 10 cm could not predict the early breakthrough of the metabolite after the first application. The modelling still results in a time delay of around one year, even if an increased dispersion length is considered. However, similar concentrations are still predicted when the daily concentrations are aggregated to longer time periods (see later in this section). In contrast to the standard FOCUS parametrisation, the simulation runs with PELMO using the dynamic macropore module do well capture the early breakthrough of the metabolite CyPM and its maximum measured concentrations. Nevertheless, the model results using the dynamic macropore module temporarily overestimates the leaching, which is reflected in high simulated metabolite concentrations between the measured peaks during the experiment.

The leaching pattern demonstrates that the three model runs with different variations of dynamic macropore flow (2-5 % / 4-8 % / 5-15 %) produce similar results regarding maximum concentrations. However, during the first application period the leaching patterns show some differences in the height of predicted concentrations. Since it is rather difficult to find the best model fit based on the visual, an additional statistical analysis was performed (see the end of this section).

Figure 26: Measured and modelled CyPM concentrations in the percolate (drainage) at 100 cm at Estrup PLAP site with logarithmic scale

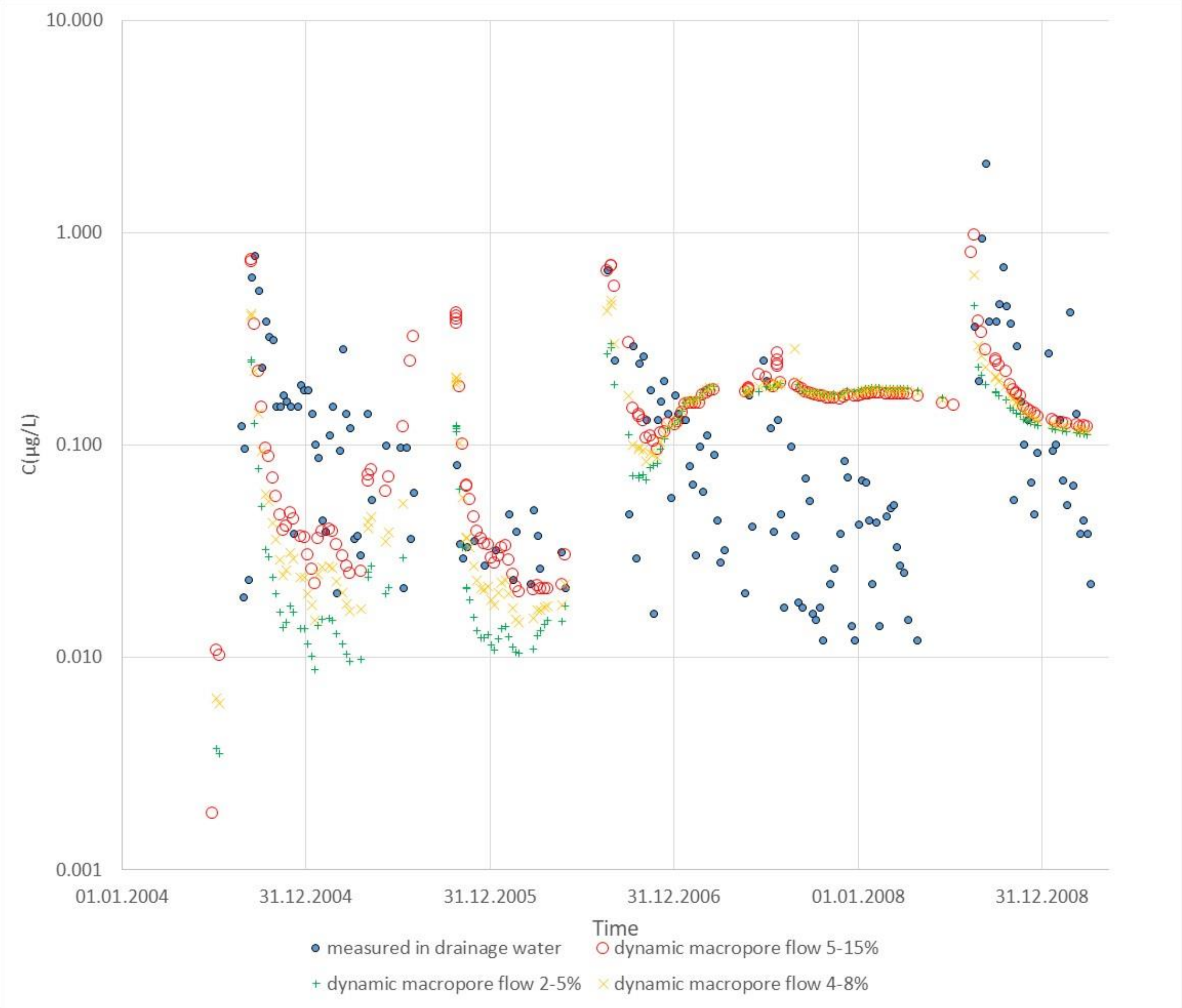
Different dynamic macropore flow variations have been modelled with PELMO and compared to FOCUS standard model parametrisation and an increased dispersion length. The rates in the legend refer to minimum and maximum fractions of precipitation in the dynamic macropore module.



Source: own illustration, Fraunhofer IME.

Figure 27: Measured and modelled azoxystrobin concentrations in the percolate (drainage) at 100 cm at Estrup PLAP site with logarithmic scale

Three different dynamic macropore flow variations have been modelled with PELMO and are compared to experimental results. The rates in the legend refer to minimum and maximum fractions of precipitation used in the dynamic macropore module.

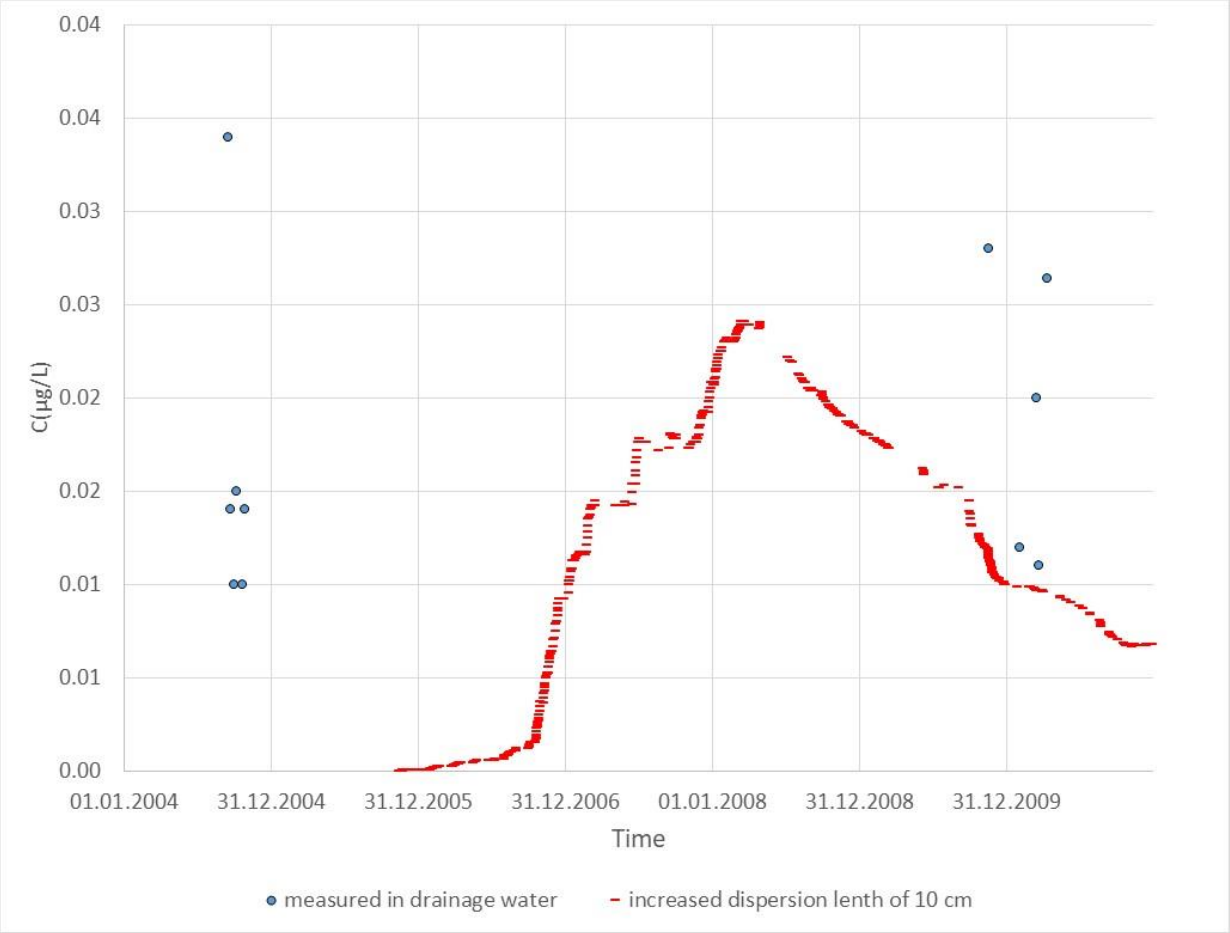


Source: own illustration, Fraunhofer IME

For Silstrup, the standard FOCUS simulations with PELMO based on chromatographic flow did not predict any concentrations of azoxystrobin in the percolate and results are therefore not presented in the following. The simulation run with an increased dispersion length of 10 cm (red hyphen in Figure 28 did not correctly predict the temporal dynamic of the leachate concentrations but calculated overall similar concentrations as measured in the PLAP experiment. The four model runs with PELMO using the dynamic macropore module overestimated the concentrations of the active substance in the leachate by more than one order of magnitude, but at least the two peaks in 2004 and 2010 after application were correctly captured. The peak between in 2005 simulated by the model was not observed in the field (see Figure 29 and Figure 30).

Figure 28: **Measured and modelled azoxystrobin concentrations in the percolate (drainage) at 100 cm at Silstrup PLAP site**

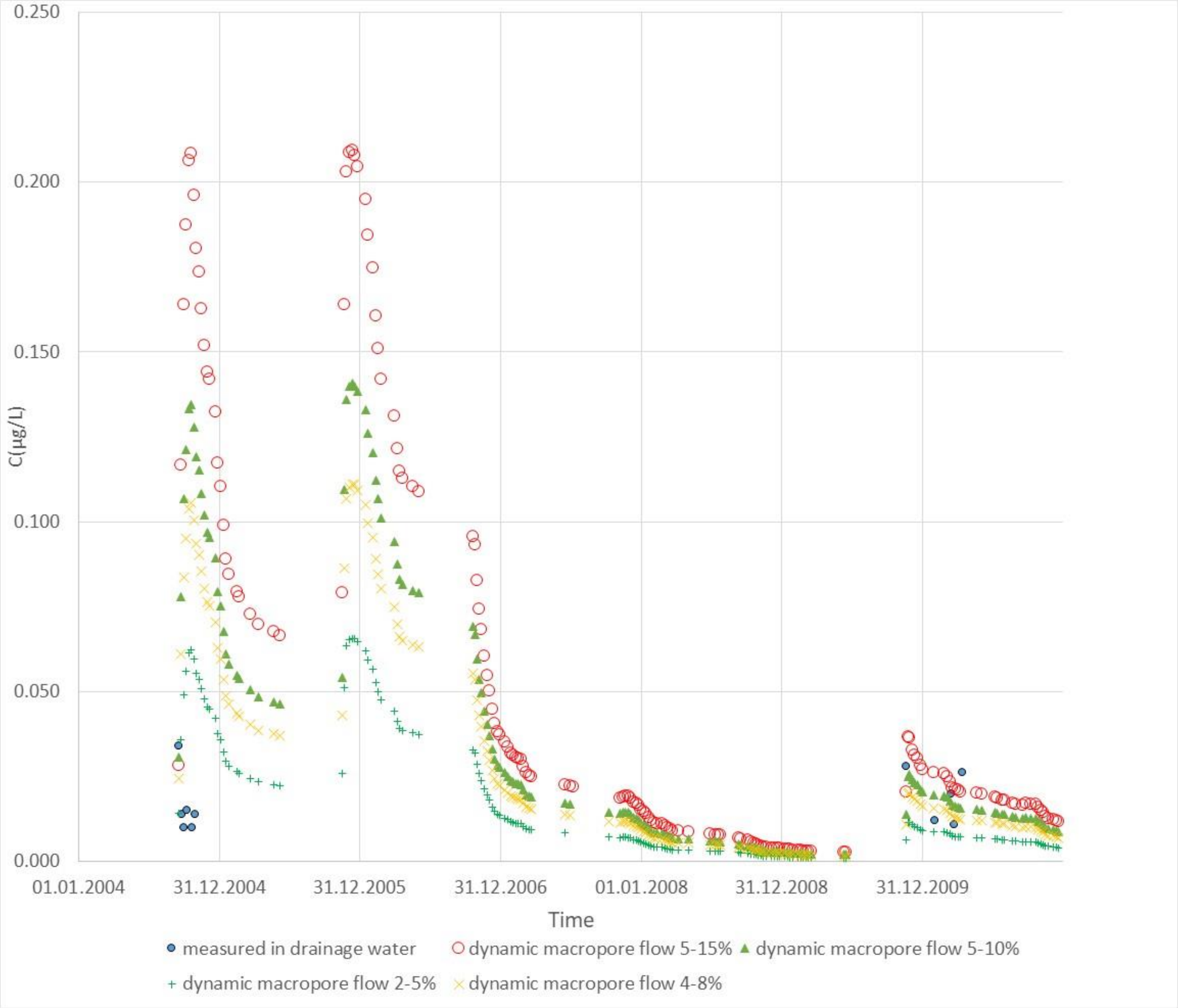
Results from a PELMO simulation using the FOCUS parametrisation with an increased dispersion length of 10 cm are compared to measured concentrations.



Source: own illustration, Fraunhofer IME

Figure 29: Measured and modelled azoxystrobin concentrations in the percolate (drainage) at 100 cm at Silstrup PLAP site

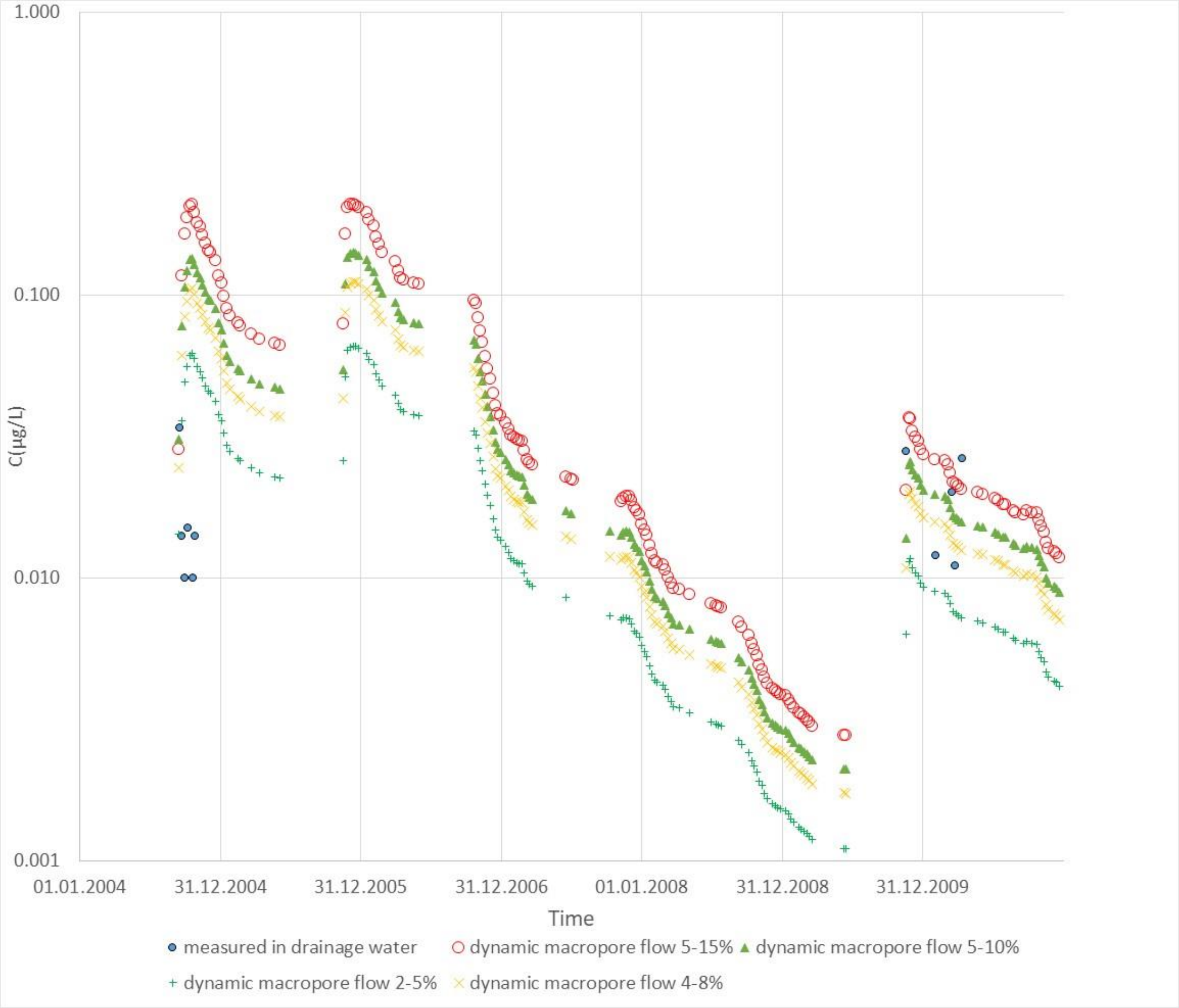
Different dynamic macropore flow variations have been modelled with PELMO and are compared to measured concentrations. The rates in the legend refer to minimum and maximum fractions of precipitation used in the dynamic macropore flow model approach.



Source: own illustration, Fraunhofer IME

Figure 30: Measured and modelled azoxystrobin concentrations in the percolate (drainage) at 100 cm at Silstrup PLAP site in logarithmic scale

Different dynamic macropore flow variations have been modelled with PELMO and are compared to measured concentrations. The rates in the legend refer to minimum and maximum fractions of precipitation used in the dynamic macropore flow model approach.

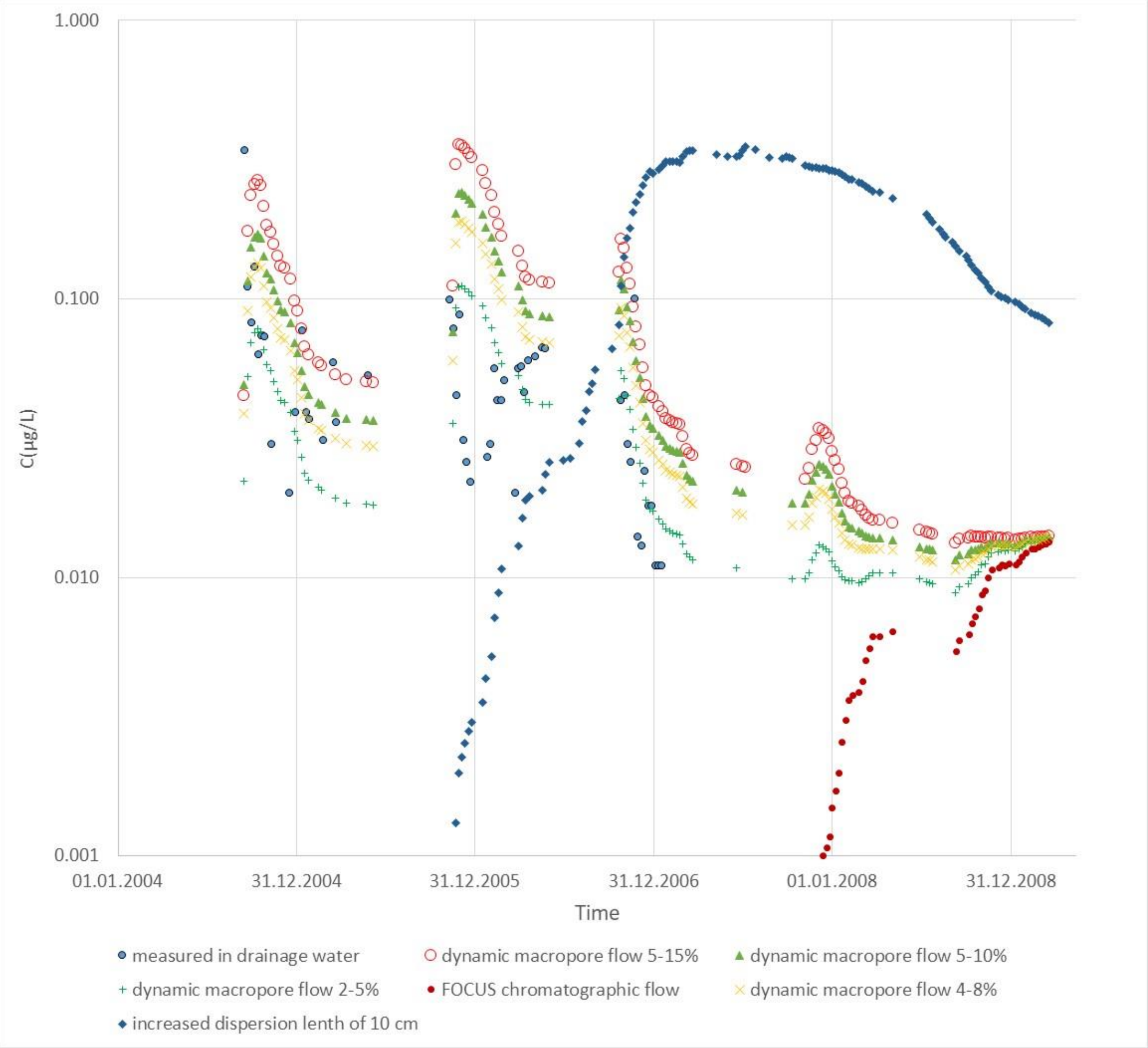


Source: own illustration, Fraunhofer IME

The respective modelling results for the metabolite CyPM are presented in Figure 31. In the PELMO simulation run based on FOCUS standard parametrisation (chromatographic flow only, dispersion length of 5 cm) the measured concentrations are significantly underestimated. In the simulation run considering an extended dispersion length of 10 cm the height of the measured concentrations could be reached. However, the temporal breakthrough of the metabolite significantly differs from the experiment, and the model cannot capture the three measured peaks. In contrast, the PELMO simulation runs using the dynamic macropore module show a comparable behaviour between modelled and measured concentrations. Both, the height and dynamic of the drainage concentration after leaching are well predicted.

Figure 31: Measured and modelled CyPM concentrations in the percolate (drainage) at 100 cm at Silstrup PLAP site in logarithmic scale

Different dynamic macropore flow variations have been modelled with PELMO and compared to FOCUS standard model parametrisation and an increased dispersion length. The rates in the legend refer to minimum and maximum fractions of precipitation used in the dynamic macropore model approach.



Source: own illustration, Fraunhofer IME

The visual comparison of measured and modelled drainage concentrations of azoxystrobin and its metabolite CyPM based on different modelling routines with PELMO shows that the FOCUS standard modelling routine considering chromatographic flow does not capture the height and break-through of both compounds at the two PLAP sites Estrup and Silstrup. An increase in the dispersion length causes increased percolation concentrations and earlier breakthrough times, whereby the concentration curves after application of the active ingredient cannot be covered approximately. The introduction of the dynamic macropore model, on the other hand, shows well adapted concentration series, which are closed in time to the measured concentrations. It is still rather difficult to find the best fit from the different used model variations based on the presented graphical outputs. Therefore, a statistical analysis was performed and is presented in the following.

Comparison of results for azoxystrobin/CyPM at Estrup and Silstrup

In the following statistical results are presented related to the previous simulations and diagrams. All concentrations from the PLAP experiment and from PELMO simulations are based on weekly aggregation.

Table 22 shows the comparison between measured and simulated maximum weekly concentrations. At Estrup, the leaching of the active substance azoxystrobin and its metabolite CyPM can be best described based on the variation with high dynamic macropore fractions in soil (see numbers marked with an asterisk in the table). In contrast, at Silstrup, the leaching of both compounds is better represented by the model variations with low or moderate dynamic macropore flow fraction in soil.

Table 22: Comparison of weekly maximum concentrations (µg/L) measured in PLAP and simulated with PELMO

Substance	Site	Measured in PLAP	Macropore flow 2-5%	Macropore flow 4-8%	Macropore flow 5-10%	Macropore flow 5-15%	FOCUS standard^
Azoxystrobin	Estrup	1.4	0.676	1.080	**1.375***	2.045	0.008
CyPM	Estrup	2.1	0.770	0.921	1.130	**1.595***	0.800
Azoxystrobin	Silstrup	0.034	**0.066***	0.111	0.141	0.210	0.000
CyPM	Silstrup	0.150	**0.112***	**0.190***	0.241	0.358	0.013

* considered to be in good agreement ^ no macropore simulation, dispersion length 5 cm

Table 23 shows the comparison between measured and simulated weekly 80th percentile concentrations. At Estrup, the leaching of the parent compound can be best described based on the PELMO variations with high or moderate dynamic macropore flow fractions in soil (see the asterisks in the table). At E strup, the 80th percentile concentrations of the metabolite CyPM are always overestimated by the model even when performing simulations without macropore flow (standard PELMO module). Consequently, at Silstrup, the leaching of active substance azoxystrobin and its metabolite CyPM is better represented based on the PELMO variations with low or moderate dynamic macropore flow fractions in soil.

Table 23: Comparison of weekly 80th percentile concentrations (µg/L) measured in PLAP and simulated with PELMO

Substance	Site	Measured in PLAP	Macropore flow 2-5%	Macropore flow 4-8%	Macropore flow 5-10%	Macropore flow 5-15%	FOCUS standard^
Azoxystrobin	Estrup	0.094	0.034	0.061	**0.078***	**0.102***	0.003
CyPM	Estrup	0.176	0.424	0.443	0.464	0.482	0.398
Azoxystrobin	Silstrup	0.026	**0.036***	0.061	0.077	0.110	0
CyPM	Silstrup	0.064	**0.042***	**0.071***	0.088	0.117	0.010

* considered to be in good agreement ^ no macropore simulation, dispersion length 5 cm

Table 24 shows the comparison between measured and simulated weekly median concentrations. At Estrup, the leaching of the parent compound can be best described based on the model variation with high macropore flow fractions in soil (see the asterisks in the table). At Estrup, the median concentration of the metabolite CyPM is always overestimated. At Silstrup, the leaching of the parent compound is better represented by the model variation with moderate macropore flow fractions in soil. However, the leaching of metabolite CyPM is underestimated with the standard PELMO version. The best fit is achieved with the PELMO variation with a high dynamic macropore flow portion.

Table 24: Comparison of weekly 80th median concentrations (µg/L) measured in PLAP and simulated with PELMO

Substance	Site	Measured in PLAP	Macropore flow 2-5%	Macropore flow 4-8%	Macropore flow 5-10%	Macropore flow 5-15%	FOCUS standard^
Azoxystrobin	Estrup	0.039	0.013	0.022	0.028	**0.036***	0.001
CyPM	Estrup	0.068	0.180	0.180	0.180	0.185	0.169
Azoxystrobin	Silstrup	0.014	0.008	**0.014***	**0.017***	0.022	0.000
CyPM	Silstrup	0.045	0.015	0.021	**0.025***	**0.032***	0.001

* considered to be in good agreement ^ no macropore simulation, dispersion length 5 cm

The question of which dynamic macropore model variation best reflects the measurement results depends on the evaluation of the results. Irrespective of this, the detections of the active substance azoxystrobin and partly of the metabolite CyPM in Estrup tend to be calculated by high percentages and in Silstrup by low to moderate percentages of macropore flow. Overall, it can be concluded that the differences between the PELMO's variations are smaller than differences between the locations in the PLAP experiment. Looking at all results, the variation with 4 % static and 8 % dynamic macropore flow seems to be a compromise for the parametrisation of macropore flow in PELMO.

4.3.4.3 Comparison of measured and modelled lysimeter results

The data from several lysimeter studies in non-sandy soils was published in Kördel et al. (2003). Outdoor plot and lysimeter experiments with tracers (bromide, dye and particles) and different pesticides were performed to investigate preferential flow and transport by macropores and to simulate these processes with leaching models. The existing lysimeter concept according to BBA (1990) was extended by using large suction plates. The experiments finally confirmed the importance of macropore flow for a fast transport of pesticides in silty soils. The authors elucidated the high variability of macropore flow and transport in time and space combined with a co-transport for poorly soluble pesticides. Significant differences were elaborated between the two lysimeter technique with and without suction plates. The amount of leachate and pesticide concentrations were significantly lower from samplings of the suction plates. During this project, macropore flow was included as a process for modelling in PELMO based on a comparison with the experimental data set.

The idea of considering this lysimeter data again in this project was to provide an additional preferential flow calibration for PELMO based on the new dynamic macropore modelling approach in comparison with the calibration results based on the PLAP data set. The experimental data set is suitable for this purpose, because it consists of several lysimeter cores using silty soils to explicitly study preferential flow in non-sandy soils. One of the soils used in the project was the 'Ebbinghof' soil. This soil was selected for comparing the calibrated macropore flow in PELMO with the measured lysimeter data, because its soil texture belongs to class M3, which considers potential high macropore flow. This facilitates a comparison with the PLAP sites Estrup and Silstrup, which both belong to the same macropore flow class.

Information about the soil characteristic of 'Ebbinghof' is provided in Table 25. The surface areas of the lysimeter cores were 1 m^2.

Table 25: Characteristics of the soil profile Ebbinghof (Kördel et al. 2003)

Horizon (cm)	Sand (%)	Silt (%)	Clay (%)	C_{org} (%)	Density (g/cmt³)	Porosity (%)	Degradation factor
0-30	14.1	58.0	28.0	1.90	1.21	54.3	1.0
30-60	21.1	50.4	28.5	0.99	1.19	55.1	0.5
60-80	22.9	46.3	30.8	0.66	1.25	52.6	0.3
80-100	34.0	44.3	21.7	0.08	1.69	36.3	0.3

Two pesticides were selected for the comparison: isoproturon and terbutyhlazine. With regard to the crop specific input data the default values of PELMO were used. The necessary information on emergence, maturation and harvest was taken from the experimental data (see Table 26). The weather data was recorded during the experiment at the Schmallenberg lysimeter station where the lysimeters study was performed.

Table 26: Information on crop rotation in the lysimeter study (Kördel et al. 2003)

Parameter	Emergence	Maturation	Harvest
Winter wheat	19/10/1998	05/05/1999	05/05/1999
Maize	19/05/1999	15/09/1999	25/05/1999
Winter wheat	24/10/2000	05/05/2000	05/05/2000
Maize	19/05/2000	15/09/2000	25/09/2000
Winter wheat	28/09/2000	25/05/2001	25/05/2001

For the comparison of modelled and measured results three different PELMO model variations were used:

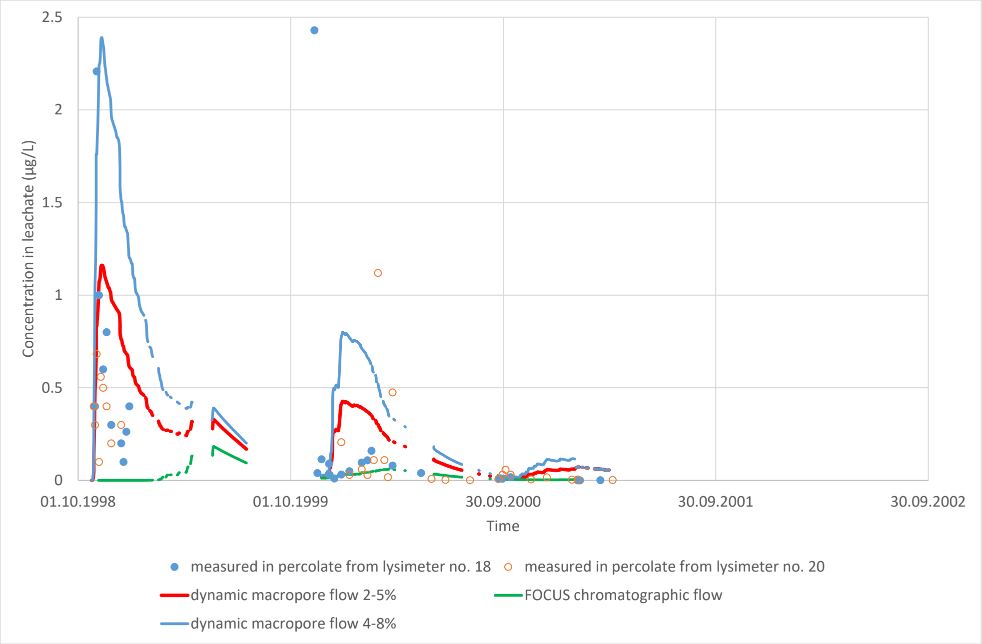
- Standard FOCUS PELMO (chromatographic flow only; without macropore flow)
- PELMO including macropore flow (4 % static and 8 % dynamic maximum macropore flow)
- PELMO including macropore flow (2 % static and 5 % dynamic maximum macropore flow)

The results of the comparison are presented in Figure 32 and Figure 33 for isoproturon and terbuthylazine, respectively.

Table 27 shows a statistical description of the comparison between the measured percolate concentrations and the PELMO simulations.

Figure 32: Measured and modelled isoproturon concentrations (µg/L) in the percolate of a lysimeter at 1 m depth with Ebbinghof soil

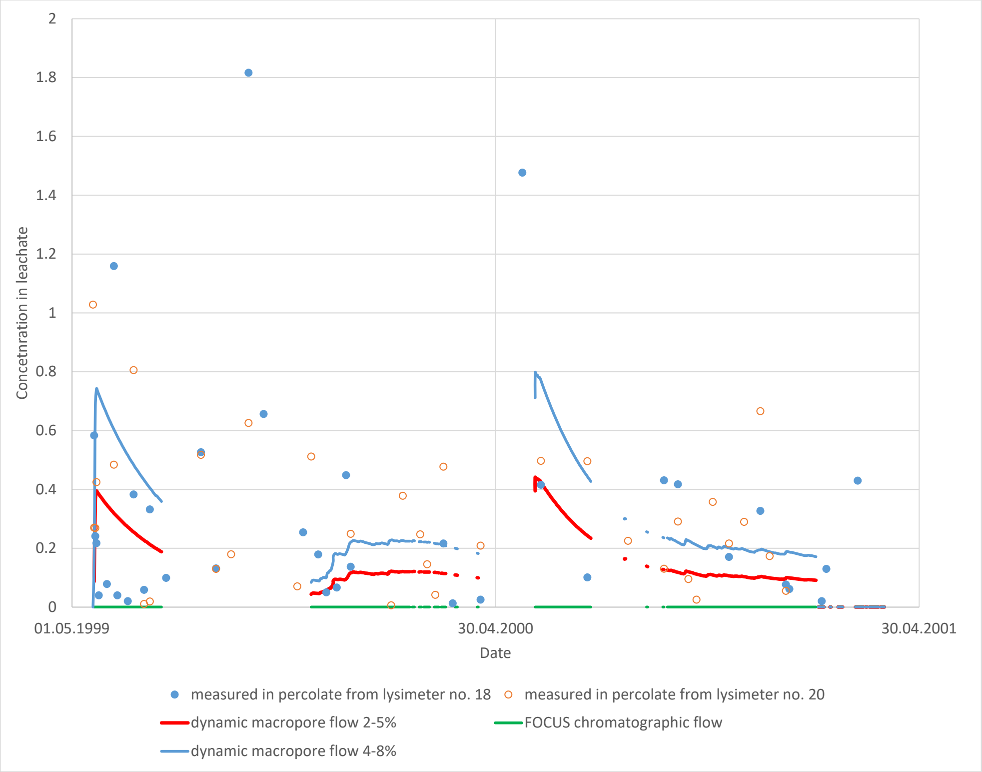
Three different macropore flow variations have been modelled with PELMO. The numbers in the legend refer to minimum and maximum fractions of dynamic macropore flow.



Source: own illustration, Fraunhofer IME

Figure 33: Measured and modelled terbuthylazine concentrations (µg/L) in the percolate of a lysimeter at 1 m depth with Ebbinghof soil

Three different macropore flow variations have been modelled with PELMO. The numbers in the legend refer to minimum and maximum fractions of dynamic macropore flow.



Source: own illustration, Fraunhofer IME

Table 27: Statistical evaluation of the comparison between the measured and calculated daily percolate concentrations at 1 m (µg/L

Bold values refer to acceptable agreement between the pesticide concentrations from experiment and from simulations.

Endpoint	Active substance	Measured percolate in lysimeter 18 [µg/L]	Measured percolate in lysimeter 20 [µg/L]	FOCUS chromato–graphic flow [µg/L]	Dynamic macropore flow 2-5% [µg/L]	Dynamic macropore flow 4-8% [µg/L]
Maximum	isoproturon	5.72	1.12	0.18	**1.16**	**2.39**
Maximum	terbuthylazine	40.97	8.04	0.00	0.44	0.80
80th percentile	isoproturon	0.52	0.42	0.06	**0.41**	0.75
80th percentile	terbuthylazine	0.48	0.51	0.00	0.24	**0.45**
Arith. mean	isoproturon	0.56	0.23	0.03	**0.26**	**0.47**
Arith. mean	terbuthylazine	1.48	0.67	0.00	0.14	0.27
Median	isoproturon	0.11	0.11	0.02	**0.19**	0.25
Median	terbuthylazine	0.22	0.27	0.00	0.11	**0.21**

The results of the comparison analysis can be summarised as follows:

- Considering the maximum isoproturon leachate concentrations in both macropore flow model variations calculated concentrations are obtained in the range of experimental data. The FOCUS standard modelling approach does not capture the measured concentrations. In contrast, the maximum terbuthylazine concentrations are clearly underpredicted by all model variations.
- When comparing the 80th percentiles of the daily leachate concentrations the situation improved. For both active substances the simulated values by using the dynamic macropore flow model are in the range of the experimental results: For isoproturon the variation with 2 % to 5 % dynamic macropore flow fraction performs best, whereas for terbuthylazine the variation with 4 % to 8 % dynamic macropore flow fraction shows a better agreement. In contrast, the standard FOCUS PELMO version with chromatographic flow only wasn’t able to reproduce the experimental data for both compounds.
- When comparing the median values of the daily leachate concentrations the same results were found as for the 80th percentile: For isoproturon the variation with 2 % to 5 % dynamic macropore flow fraction performs best, whereas for terbuthylazine the variation with 4 % to 8 % macropore flow fraction shows a better agreement. In contrast, the standard FOCUS PELMO version with chromatographic flow only wasn’t able to reproduce the experimental data for both compounds.

It can be concluded that the model version without macropores flow wasn’t able to capture the result of the lysimeter studies. There was no clear evidence for one of the two PELMO model variations with low to medium dynamic macropore flow to capture the lysimeter results. The isoproturon leaching experiment was better captured by modelling with the minimum and maximum macropore flow fractions of 2 % and 5 %, whereas the terbuthylazine experiment could be better reproduced with the minimum and maximum macropore flow fractions of 4 % and 8 %.

This analysis leads to reasonable results that preferential flow occurred in the lysimeter experiments with silty soils according to Kördel at al. (2003). The leachate concentrations and pattern can be reproduced by modelling with PELMO only if the dynamic macropore flow module is used in parallel to the standard chromatographic flow module. The comparison showed that a calibration with low (2-5 %) to medium (4-8 %) macropore flow in principle provides acceptable results for two other active substances, weather situations and another soil referring to texture class M3.

Those results are mainly in line with the calibration analysis for azoxystrobin and CyPM at two PLAP sites, even though some uncertainty about the best parametrisation remain. Considering all results from both calibration analysis the model variation with 4 % static and 8 % dynamic macropore flow seems to be a compromise for the parametrisation of preferential flow in PELMO.

4.3.4.4 Comparison of PELMO with FOCUS MACRO simulations

In this section an attempt is made to verify how far the different macropore flow modules in PELMO lead to similar results as respective simulations with FOCUS MACRO. As the FOCUS groundwater approach only implemented Châteaudun as preferential flow scenario (European Commission 2014), results are provided for this location, only. An overview about the properties of the FOCUS Châteaudun soil profile is given in Table 28.

Because the results of this evaluation strongly depend on pesticide properties and application pattern a reasonable range of situations with nine fictive compounds and two different application patterns were considered in this calibration. The properties of the dummy compounds differ in their sorption constants (K_{foc}) and their degradation rates in soil ($DegT_{50}$) (see Table 29).

Table 28: Characteristic of the FOCUS Châteaudun soil profile (macropore flow class M 3)

Horizon [-]	Depth [cm]	Type [-]	Texture < 2 µm [%]	Texture 2-50 µm [%]	Texture >50 µm [%]	OC [%]	Density [kg/L]	Ksat [µm/s]	FC [L/L]	WP [L/L]
Ap	0-25	silty clay loam	30	67	3	1.39	1.30	20.0	0.374	0.253
B1	25-50	silty clay loam	31	67	2	0.93	1.41	30.0	0.372	0.235
B2	50-60	silt loam	25	67	8	0.70	1.41	50.0	0.372	0.235
II C1	60-100	limestone	26	44	30	0.30	1.37	12.0	0.386	0.185
II C1	100-120	limestone	26	44	30	0.30	1.37	12.0	0.386	0.185
II C2	120-190	limestone	24	38	38	0.27	1.41	9.1	0.417	0.116

All simulations were performed in maize and winter cereals over a period of 26 years including a warming up period of 6 years and with annual applications one day before emergence of the crop. In general, an application rate of 200 g/ha was chosen. However, for some compounds the application rate was adapted to achieve a range of leaching concentrations, which do not exceed one order of magnitude above or below the groundwater limit value of 0.1 µg/L.

Table 29: **Properties of the nine fictive compounds used for the calibration**

Crop	K_{foc} [L/kg]	$DegT_{50}$ [d]	Application rate [kg/ha]
Winter cereals	15	5	0.20
Winter cereals	15	20	0.02
Winter cereals	15	80	0.01
Winter cereals	30	10	0.20
Winter cereals	60	20	0.20
Winter cereals	60	80	0.02
Winter cereals	120	40	0.20
Winter cereals	240	80	0.20
Winter cereals	480	160	0.20
Maize	15	5	5.00
Maize	15	20	0.02
Maize	15	80	0.01
Maize	30	10	0.20
Maize	60	20	0.20
Maize	60	80	0.02
Maize	120	40	0.20
Maize	240	80	0.20
Maize	480	160	0.20

Five PELMO model variations regarding different dispersion lengths in a range of 5 cm (standard FOCUS PELMO) to 20 cm were considered (Table 30). In addition, three PELMO model variations with reduced field capacities of 10 %, 25 % and 50 % (Table 31) and three model variations with dynamic macropore flow module were considered (Table 32). Two of the last model variations, which have been used to calibrate PELMO based on the PLAP data, represent a minimum and maximum of 2-5 % and 4-8 % of dynamic preferential flow with a macropore compartment defined until a soil depth of 80 cm. Another model variation of 2-5 % dynamic preferential flow was calculated with a macropore compartment defined until a soil depth of 60 cm (see chapter 4.3.4.1). For all model runs, the 80th percentile of annual percolate concentration at 1 m soil depth was selected for a comparison with MACRO simulations. The results are presented in order from minimum to maximum leachate concentration based on results for the MACRO Châteaudun scenario (see Table 30, Table 31 and Table 32).

Table 30: Comparison of the 80th temporal percentile of percolate concentrations

PELMO variations with adjusted dispersion lengths considering simulations in winter cereals (WC) and maize (MZ).

K_{foc} [L/kg]	$DegT_{50}$ [d]	Crop [-]	FOCUS MACRO version 5.5.4 [µg/L]	PELMO 5 cm Disp length [µg/L]	PELMO 7.5 cm Disp length [µg/L]	PELMO 8.5 cm Disp length [µg/L]	PELMO 10 cm Disp length [µg/L]	PELMO 20 cm Disp length [µg/L]
30	10	MZ	0.005	0.001	0.002	0.003	0.004	0.016
480	160	WC	0.008	0.001	0.002	0.004	0.010	0.124
15	5	MZ	0.009	0.001	0.004	0.008	0.016	0.234
480	160	MZ	0.012	0.005	0.019	0.028	0.044	0.223
60	20	MZ	0.015	0.004	0.009	0.012	0.019	0.087
240	80	MZ	0.017	0.008	0.023	0.032	0.047	0.220
120	40	MZ	0.019	0.006	0.018	0.025	0.038	0.172
240	80	WC	0.019	0.002	0.009	0.014	0.023	0.190
15	5	WC	0.022	0.008	0.032	0.049	0.079	0.394
120	40	WC	0.027	0.004	0.015	0.021	0.034	0.220
15	20	MZ	0.028	0.021	0.030	0.034	0.038	0.059
30	10	WC	0.031	0.004	0.025	0.039	0.065	0.468
60	20	WC	0.035	0.004	0.015	0.021	0.036	0.262
15	20	WC	0.139	0.065	0.110	0.136	0.173	0.415
60	80	MZ	0.174	0.166	0.218	0.232	0.245	0.357
60	80	WC	0.300	0.188	0.251	0.277	0.307	0.490
15	80	MZ	0.417	0.352	0.375	0.381	0.400	0.442
15	80	WC	0.949	0.654	0.705	0.723	0.700	0.990
Geometric mean of all results			0.038	0.011	0.028	0.038	0.055	0.219
Correlation coefficient (R^2)				0.992	0.991	0.990	0.981	0.874

Table 31: Comparison of the 80th temporal percentile of percolate concentrations

PELMO variations with adjusted (reduced) field capacities considering simulations in winter cereals (WC) and maize (MZ).

K_{foc} [L/kg]	$DegT_{50}$ [d]	Crop [-]	FOCUS MACRO version 5.5.4 [µg/L]	PELMO no reduction [µg/L]	PELMO 10% reduction [µg/L]	PELMO 25% reduction [µg/L]	PELMO 50% reduction [µg/L]
30	10	MZ	0.005	0.001	0.001	0.002	0.005
480	160	WC	0.008	0.001	0.0003	0.008	0.003
15	5	MZ	0.009	0.001	0.002	0.008	0.045
480	160	MZ	0.012	0.005	0.006	0.001	0.013
60	20	MZ	0.015	0.004	0.005	0.007	0.015
240	80	MZ	0.016	0.008	0.009	0.011	0.019
120	40	MZ	0.019	0.006	0.007	0.010	0.018
240	80	WC	0.019	0.002	0.003	0.005	0.011
15	5	WC	0.022	0.008	0.013	0.030	0.150
120	40	WC	0.027	0.004	0.005	0.008	0.018
15	20	MZ	0.028	0.021	0.027	0.040	0.069
30	10	WC	0.031	0.004	0.006	0.013	0.044
60	20	WC	0.035	0.004	0.006	0.010	0.028
15	20	WC	0.139	0.065	0.083	0.126	0.315
60	80	MZ	0.174	0.166	0.191	0.223	0.289
60	80	WC	0.300	0.188	0.212	0.253	0.332
15	80	MZ	0.417	0.352	0.387	0.443	0.522
15	80	WC	0.949	0.654	0.700	0.776	0.963
Geometric mean of all results			0.038	0.011	0.013	0.022	0.048
Correlation coefficient (R^2)				0.992	0.991	0.989	0.975

As expected, increasing dispersion lengths or reduced field capacities in the PELMO simulations always lead to increased percolate concentrations. The best agreement between MACRO and modified PELMO simulations was found for a dispersion length of 8.5 cm when the geometric mean value of all 18 modelling results is compared (see last row in Table 30). And the best agreement between MACRO and modified PELMO was found for a reduced field capacity by 25 % and 50 % when the geometric mean value of all 18 modelling runs is compared (see last row in Table 31).

Table 32: Comparison of the 80th temporal percentile of percolate concentrations

PELMO variations with dynamic macropore flow considering simulations in winter cereals (WC) and maize (MZ). In the table the minimum and maximum percentages refer to the fraction of macropore flow related to the total water flux in soil. Calculations were performed assuming macropore lengths of 60 cm and 80 cm, respectively.

K_{foc} [L/kg]	$DegT_{50}$ [d]	Crop [-]	FOCUS MACRO version 5.5.4 [µg/L]	PELMO no dynamic macropore [µg/L]	PELMO dynamic macropore flux 2-5% length 80 cm [µg/L]	PELMO dynamic macropore flux 4-8% length 80 cm [µg/L]	PELMO dynamic macropore flux 2-5% length 60 cm [µg/L]
30	10	MZ	0.005	0.001	0.071	0.130	0.013
480	160	WC	0.008	0.001	0.067	0.125	0.012
15	5	MZ	0.009	0.001	1.455	2.653	0.127
480	160	MZ	0.012	0.005	0.245	0.433	0.081
60	20	MZ	0.015	0.004	0.118	0.212	0.032
240	80	MZ	0.016	0.008	0.243	0.433	0.081
120	40	MZ	0.019	0.006	0.176	0.315	0.061
240	80	WC	0.019	0.002	0.068	0.125	0.015
15	5	WC	0.022	0.008	0.126	0.216	0.039
120	40	WC	0.027	0.004	0.076	0.141	0.017
15	20	MZ	0.028	0.021	0.042	0.068	0.030
30	10	WC	0.031	0.004	0.015	0.243	0.026
60	20	WC	0.035	0.004	0.105	0.194	0.021
15	20	WC	0.139	0.065	0.085	0.108	0.076
60	80	MZ	0.174	0.166	0.204	0.233	0.199
60	80	WC	0.300	0.188	0.219	0.243	0.202
15	80	MZ	0.417	0.352	0.360	0.360	0.358
15	80	WC	0.949	0.654	0.657	0.661	0.655
Geometric mean of all results			0.038	0.011	0.138	0.244	0.056
Correlation coefficient (R^2)				0.992	0.287	0.054	0.972

The results further show that according to average annual leachate concentrations an increased dispersion length of 8.5 cm in PELMO leads to modelling results, which are much more comparable to MACRO than reducing the field capacity or any of the dynamic macropore flow modules. The main difference is that, for example, increasing the dispersion length still leads to a significant range of concentrations dependent on the compound properties and crops (from 0.003 µg/L to 0.723 µg/L). In comparison, the range of concentrations from MACRO simulations is 0.005 µg/L to 0.949 µg/L close to PELMO. In contrast, the respective range of concentrations from the macropore flow variation (4-8 %, 80 cm depth) from 0.068 µg/L to 2.653 µg/L is higher. Nevertheless, the same macropore flow variation in PELMO led to good agreement with the experience from PLAP fields, which showed a significant transport of pesticides short time after each application and more independent from the pesticide properties.

The dynamic macropore flow variation of 2-5 % and a macropore compartment until 60 cm soil depth (see last column in Table 32) fits good in comparison to MACRO results. The simulated concentrations range from 0.012 µg/L to 0.655 µg/L. The good fit with regard to concentrations and the correlation can be probably explained, because the sand content in the FOCUS MACRO Châteaudun scenario below 60 cm is significantly higher (30 %) than in the top 60 cm (3 %, 2 %, 8 %). Therefore, the chromatographic flow in deeper soil layers may be dominant below 60 cm, which is in line with the respective depth of the macropore domain in PELMO in this variation.

For this project nevertheless, the preferential flow parametrisation obtained from calibrations based on the PLAP data was further considered since the Danish PLAP fields Estrup and Silstrup may better represent German agricultural regions and soils with comparable conditions and a potential for preferential flow than the characteristic of the FOCUS Châteaudun scenario.

4.3.5 Implementation of preferential flow in GeoPELMO DE

The implementation of preferential flow in GeoPELMO DE is based on the results of the calibrations performed with the PLAP dataset (section 0) and lysimeter studies according to Kördel at al. (2003) (section 4.3.4.3). The comparison analysis provided evidence that preferential flow occurred during the PLAP and lysimeter experiments on non-sandy soils. It was further observed that the FOCUS standard parametrisation in PELMO based on chromatographic flow and an increased dispersion length are not able in most cases to cover the experimental data, mainly regarding the height and temporal breakthrough of the compounds. The measured leaching pattern could be re-modelled much more in line with the dynamic macropore module in PELMO. However, the different experiments were best represented by different parameterisations of the proportions of the static and dynamic macro flow. Therefore, a parameterisation of the macropore module is not possible that applies to all monitoring and lysimeter results investigated. As a compromise, a low to medium parameterisation of 4 % static up to a maximum of 8 % dynamic macropore flow was implemented in PELMO for the soil class M3.

Finally, in GeoPELMO DE 12.3 % of the agricultural area in Germany with agricultural soils classified as 'high macropore flow' are parametrised considering a minimum of static macropore flow of 4 % and a dynamic maximum of macropore flow of 8 % depending on the weather conditions. 52.9 % of the agricultural areas with agricultural soils classified as 'moderate macropore flow' are parametrised considering 2 % as minimum for the static macropore flow fraction and 4 % as maximum for the dynamic macropore flow fraction (corresponding to 50 % of macropore flow compared to the soil texture class with 'high macropore flow'). Finally, no macropore flow is considered for the remaining 34.8 % of the agricultural are in Germany (section 4.3.2). Macropore flow in PELMO is always considered to those percentages alongside chromatographic flow. The trigger to calculate preferential flow with the static minimum percentage in PELMO is a daily precipitation of 10 mm. Depending on the soil moisture conditions in the preceding 7 days, the dynamic proportion of macropore flow can be higher. (section 4.3.3.1).

4.4 Runoff

The runoff curve number approach (RCN) is already implemented in PELMO since FOCUS (2000) to consider and calculate runoff in groundwater exposure assessments based on four different soil hydrological classes. The curve number approach based on the FOOTPRINT soil type classification was further developed by Dubus et al. (2009) and used to implement a modelling routine for runoff for a nationwide surface water model in Germany (Bach et al. 2017). The runoff soil scenario characterisation was based on the soil map BÜK1000N (BGR 2007) and used in a first version of a nationwide groundwater model based on PELMO (Klein et al. 2019b). To keep up with current geodata developments it was decided to use the German soil map BÜK250 DE with a larger scale (BGR 2018b) in the recent project to define nationwide soil scenarios in PELMO (see section 3.3).

The RCN originally comprises surface and subsurface runoff flow. However, in all current environmental fate models (PRZM, PELMO, GLEAMS, CREAMS) the approach is related to the surface runoff only. Consequently, though GeoPELMO DE does not explicitly consider subsurface flow it is nevertheless indirectly considered by the RCN.

4.4.1 Implementation of an advanced spatial distributed runoff approach in GeoPELMO DE

The curve numbers depending on crop and soil data from the RCN approach basically originate from FOCUS (2000). The FOCUS (2000) groundwater group defined four different PRZM Soil Hydrological Groups, whereas in a research project about surface water exposure assessment for German conditions five different Soil Hydrological groups were considered (Bach et al. 2017). To consider most recent developments these five different PRZM Soil Hydrological Groups are used for the implementation of a runoff modelling routine in GeoPELMO DE. Table 33 shows the curve number values for all crop-soil combinations used for PELMO.

To run a spatial distributed leaching model like GeoPELMO DE, scenarios must be derived nationwide from the profiles of the soil map and linked to the respective runoff curve number. In a previous version of GeoPELMO DE (GISPELMO 1.0 according to Klein et al. 2019b) this link to the RCN group was based on the results of Bach et al. (2017). That was possible because in both projects (Klein et al. 2019b, Bach et al. 2017) the same soil map BÜK1000N (BGR 2007) was used. In the first step, all soil profiles of the BÜK1000N were classified according to the FOOTPRINT soil groups (FHG). Afterwards, each FHG group was attached to one of the PRZM runoff groups (A, B, B-C, C, D). The principal classification followed Centofani et al. (2008) and Dubus et al. (2009) (see Table 34).

Table 33: Runoff curve numbers [-] in PELMO (according to Bach et al. 2017)

PRZM Hydrology soil group →	A	B	BC	C	D
Fallow	77	86	89	91	94
Grass	30	58	65	71	78
Maize	62	83	86	89	93
Barley	54	70	75	80	85
Cereals	54	70	75	80	85
Sugar Beet	58	72	77	81	85
Oats	58	72	77	81	85
Rye	58	72	77	81	85
Rape	54	70	75	80	85
Soybeans	67	78	82	85	89
Potato	62	83	86	89	93
Beans	67	78	82	85	89
Vines	45	62	68	73	79
Tomatoes	62	74	78	81	86
Strawberries	58	72	77	81	85
Apples	36	60	67	73	79
Sunflower	62	83	86	89	93
Cabbage	58	72	77	81	85
Carrots	58	72	77	81	85
Bush berries	36	60	67	73	79
Citrus	36	60	67	73	79
Cotton	67	78	82	85	89
Linseed	54	70	75	80	85
Onions	58	72	77	81	85
Peas	67	78	82	85	89
Tobacco	67	78	82	85	89
Hop	36	60	67	73	79

Table 34: Description of the FOOTPRINT Hydrologic Groups (FHG) and their relation to the Parametrisation in MACRO and PRZM (Centofani et al., 2008, Table 3, p. 581f; Dubus et al. 2009).

PRZM Hydrology soil group →	Description	B*
L	Permeable, free draining soils on permeable sandy, gravelly, chalk or limestone substrates with deep groundwater (below 2 m depth).	A
M	Permeable, free draining soils on hard but fissured substrates (including karst) with deep groundwater (below 2 m depth).	B
N	Permeable, free draining soils on permeable soft loamy or clayey substrates with deep groundwater (below 2m depth).	B-C
O	Permeable soils on sandy or gravelly substrates with intermediate groundwater (at 1 - 2 m depth)	A
P	Permeable soils on soft loamy or clayey substrates with intermediate groundwater (at 1 - 2 m depth)	B-C
Q	All soils with shallow groundwater (within 1 m depth) and artificial drainage	A
R	Permeable, free draining soils with large storage, over hard impermeable substrates below 1 m depth	B
S	Permeable, free draining soils with moderate storage, over hard impermeable substrates at 0.5 - 1 m depth	B-C
T	Shallow, permeable, free draining soils with small storage, over hard impermeable substrates within 0.5 m depth	C
U	Soils with slight seasonal waterlogging ('perched' water) over soft impermeable clay substrates	B-C
V	Soils with prolonged seasonal waterlogging ('perched' water) over soft impermeable clay substrates	C
W	Free draining soils over slowly permeable substrates	B
X	Slowly permeable soils with slight seasonal waterlogging ('perched' water) over slowly permeable substrates	B or B-C
Y	Slowly permeable soil with prolonged seasonal waterlogging ('perched' water) over slowly permeable substrates	B-C
Z	All undrained peat or soils with peaty tops	D

* PRZM hydrologic soil group

Due to the fact that the BÜK250 (BGR 2018b) is used in the recent project, the FOOTPRINT approach according to Centofani et al. (2008) presented in Table 34 must be applied again to all profiles of this new soil map by assigning a corresponding PRZM Hydrologic Soil Group (PRZM HSG). The methodology is based on a decision tree with four to seven questions, which would finally lead to a complete FOOTPRINT classification. However, for runoff only the FOOTPRINT Hydrologic Group (FHG) must be defined for every soil profile. Nevertheless, not all details of the procedure were published and are currently only available to members of the former FOOTPRINT consortium. As the number of soil profiles in the BÜK250 is very extensive an automatic procedure was developed that provides the required FHG based on the information in the database. To be able to answer the questions of the FOOTPRINT classification scheme automatically for all relevant soil profiles of the BÜK250, a script in the software R was written. To get the FHG six of the seven questions have to be answered.

Depending on the combinations of different answers the FHG for each soil profile could be identified by using an Excel-flowchart developed by the FOOTPRINT working group. All possible FHG are listed in Table 34. After linking the soil profiles from the BÜK250 with the FOOTPRINT soil classification the scenarios could be implemented into GeoPELMO DE (2.0) in a similar way as in the previous version 1.0 (Klein et al. 2019b).

The resulting runoff classification based on the BÜK250 (BGR 2018b) into PRZM Soil Hydrological Groups is provided in Figure 34. Finally, 37.8 % of the German arable land is classified as SHG A, which rather represent permeable soils on sandy and gravelly substrates and are often found in Northern Germany. Furthermore, 23.7 % of arable fields are classified as SHG B, 27.5 % as SHG B-C and 11.0 % as SHG C, which are represented by different soil textures and where the tendency to runoff during heavy rainfall events more or less increases. (see Table 35).

Classification of soil profiles in FOOTPRINT Hydrologic Groups (FHG) for Runoff

An automatic R script was developed to provide the FHG according to runoff for all soil profiles from soil map BÜK250 (BGR 2018b). To get the FHG six of the seven questions have to be answered. For the classification the following six questions need to be answered:

Question 1 'Substrate type':

The substrate type is derived from every unique combination of 'GEOGEN' and 'HERK' which are attributes in the soil horizon table of the BÜK250. In the BÜK250 there are around 1200 of such combinations. The substrate type of the deepest soil layer is assigned to the whole profile. Seven different substrate types are defined.

Question 2 'Presence of artificial drains':

A hydromorphy level is assigned to every soil horizon. The options are: 0 = no hydromorphy; 1 = low hydromorphy; 2 = strong hydromorphy. All soil types with land use type 'arable' or 'permanent crops' and a beginning of hydromorphic level 2 in a soil depth less than 80 cm are assumed as 'drained'.

Question 3 'Presence of gley morphology':

Based on the results of question 2 the depth of hydromorphical traits is checked. There are three possible answers: 'begin of hydromorphy (level 1 or 2) in ≤ 40 cm soil depth'; or: 'begin of hydromorphy (level 1 or 2) in > 40-80 cm soil depth'; or: 'none of these'.

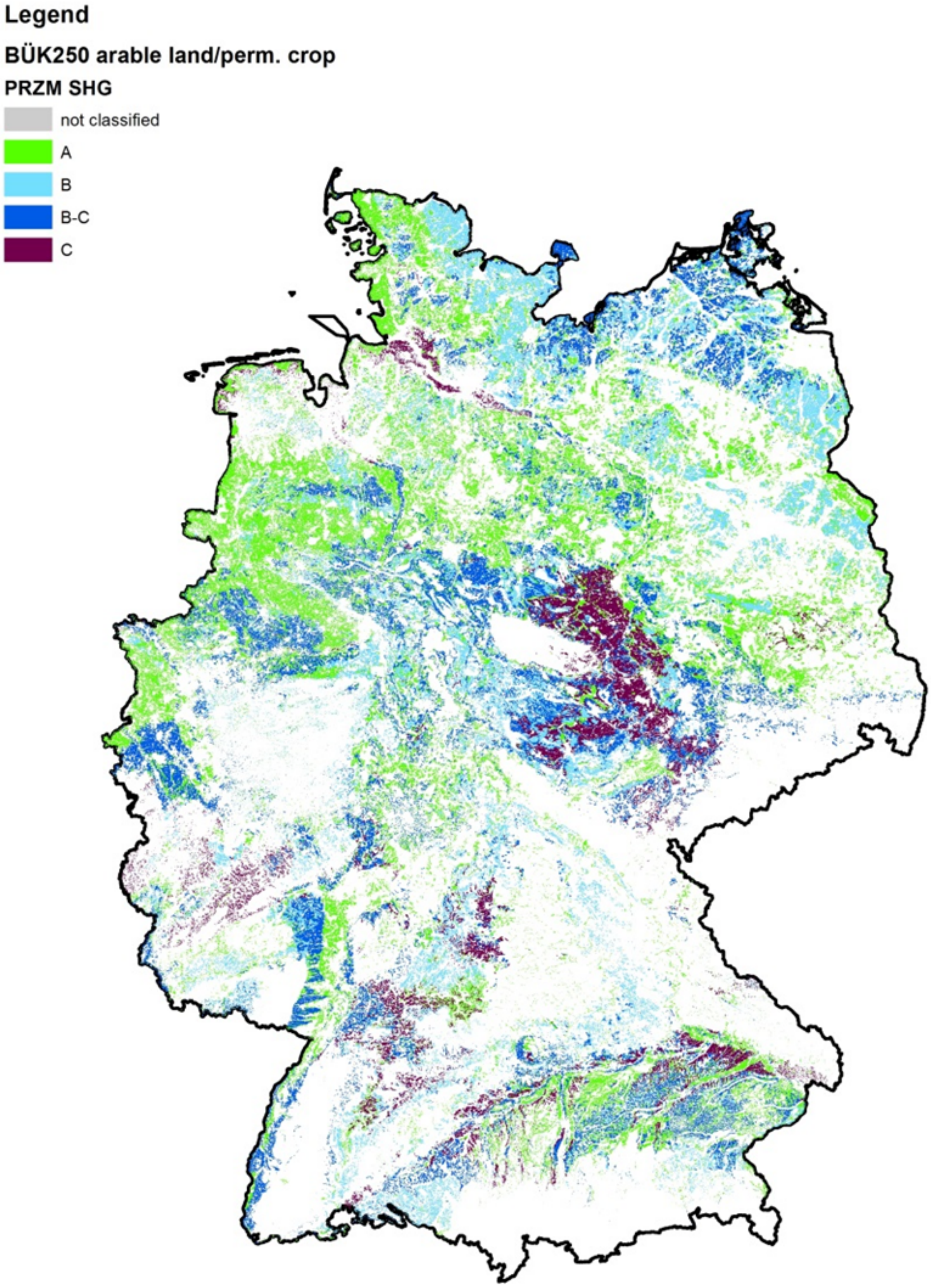
Question 4 'Presence of hard rock or rock rubble':

Firstly, every soil horizon gets the attribute '1: hard rock or rubble '(C-horizons with a prefixed 'm') or '0: other'. Secondly, the initial depth of hard rock or rubble is checked based on this information. The three possible answers are: 'begin of hardrock/rock rubble in ≤ 40 cm soil depth'; or:' begin of hard rock/rock rubble in > 40-80 cm soil depth'; or: 'none of these'.

Question 5 and 6 'Texture class of topsoil and subsoil':

The German texture classes provided in the BÜK250 are translated to the FAO soil classification (IUSS Working Group WRB 2015)

Figure 34: **Distribution of the PRZM Soil Hydrological Group (SHG) based on the BÜK250 according to the FOOTPRINT soil classification**



Source: own illustration, Fraunhofer IME (according to BGR 2018b)

Table 35: Area fractions of PRZM Soil Hydrologic Groups regarding runoff classes for arable land in Germany according to the soil map BÜK250 (BGR 2018b)

PRZM Soil Hydrologic Group (SHG) [-]	Arable area [km^2]	Arable area [%]
SHG A	40619	37.8
SHG B	25418	23.7
SHG B-C	29542	27.5
SHG C	11800	11.0

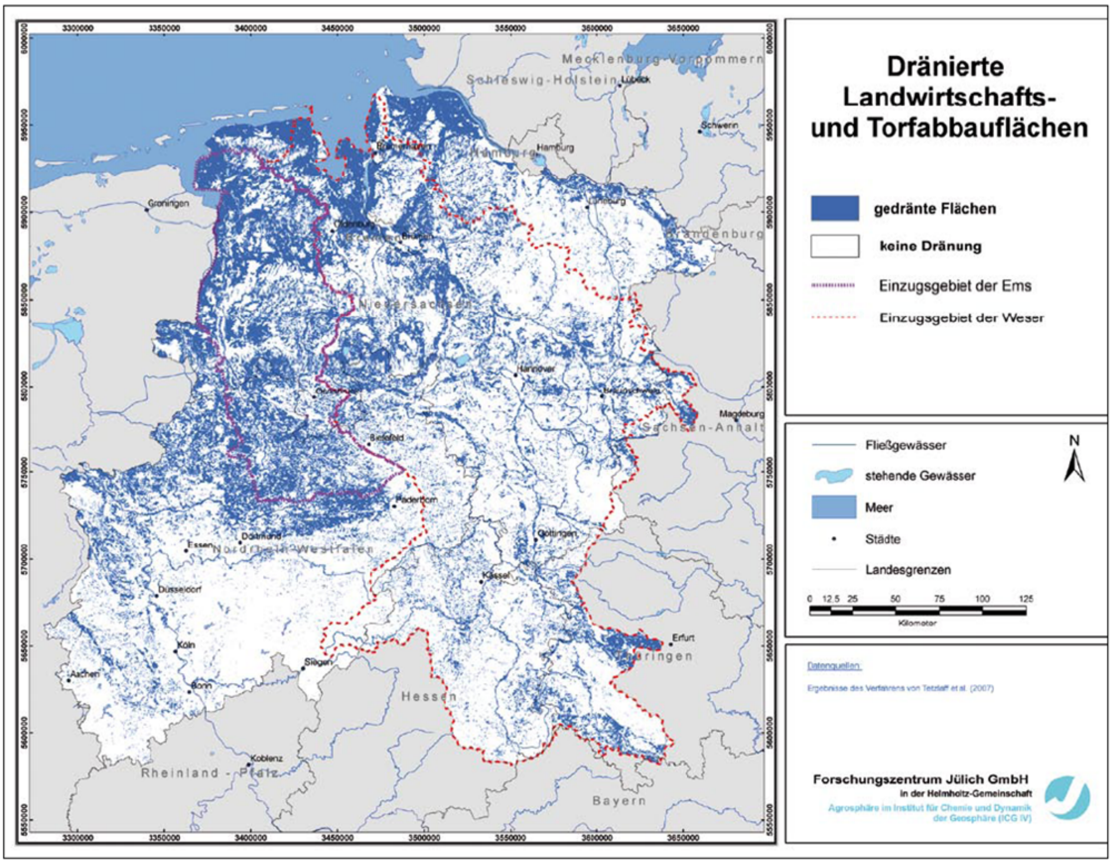
4.5 Drainage

Percolate losses due to drainage systems are currently not considered in the standard pesticide risk assessment for groundwater, because FOCUS modelling is based on a limited number of soil-climate scenarios, which cover large agricultural areas in Europe (European Commission 2014). This is different for the risk assessment for surface water where drainage is implemented in FOCUS models since 2001, because drainage is considered as possible pathway for pesticides into surface water bodies (FOCUS 2001b). It was discussed already in section 3.5 that, in contrast to a simplified scenario-based approach, spatial distributed leaching modelling may include the effect of drainage, because large parts of the agricultural area in Germany are drained, especially in the northern lowlands. Locally, a very high amount of water in the soil zone contributes to drainage flow, so this process cannot be ignored. Drainage water mostly reaches adjacent small surface water bodies and does therefore not reach groundwater via direct laminar leaching. Including the effect of artificial drainage into spatial distributed leaching modelling can increase scientific reliability for evaluating the protection level of the single FOCUS Hamburg scenario for Germany. However, it is further analysed and discussed in the following, how drainage systems and their efficiency could be considered for the calculation of nationwide percolate concentrations with GeoPELMO DE based on available geodata.

4.5.1 Available information on potentially drained areas in Northern Germany

Based on their research, Tetzlaff et al. (2008, 2009) found that artificial drainpipe installations play a major role in lowland regions in Northern Germany, but limited spatial information is available to localize such drainpipes within larger river basins. Artificially drained areas were identified at field scale in test regions in Lower Saxony by interpreting aerial photographs (Tetzlaff et al. 2008, 2009). Typical site conditions of the drained field were derived afterwards. The authors developed a GIS-based approach, which allowed the delineation of artificially drained fields by combining various site conditions like soil properties and land use types. Figure 35 shows a resulting map for the river Ems and Weser basin according to the method in Tetzlaff et al. (2008, 2009). Based on small-scale drain pipe installation maps, the approach from FZ Jülich was already applied to several federal states in Northern Germany (e.g. Wendland et al. 2015, Tetzlaff et al. 2013, 2017). Finally, maps of potentially drained areas have been made available for the project for six federal states in Northern Germany: Schleswig-Holstein, Mecklenburg-West Pomerania, Saxony, Saxony-Anhalt, Lower Saxony and North Rhine-Westphalia (Table 36).

Figure 35: Map of potentially drained areas in Lower Saxony and North Rhine-Westphalia and in the Weser river basin



Source: Tetzlaff et al. 2008, p. 16

Table 36: Availability of drainage data in Northern Germany

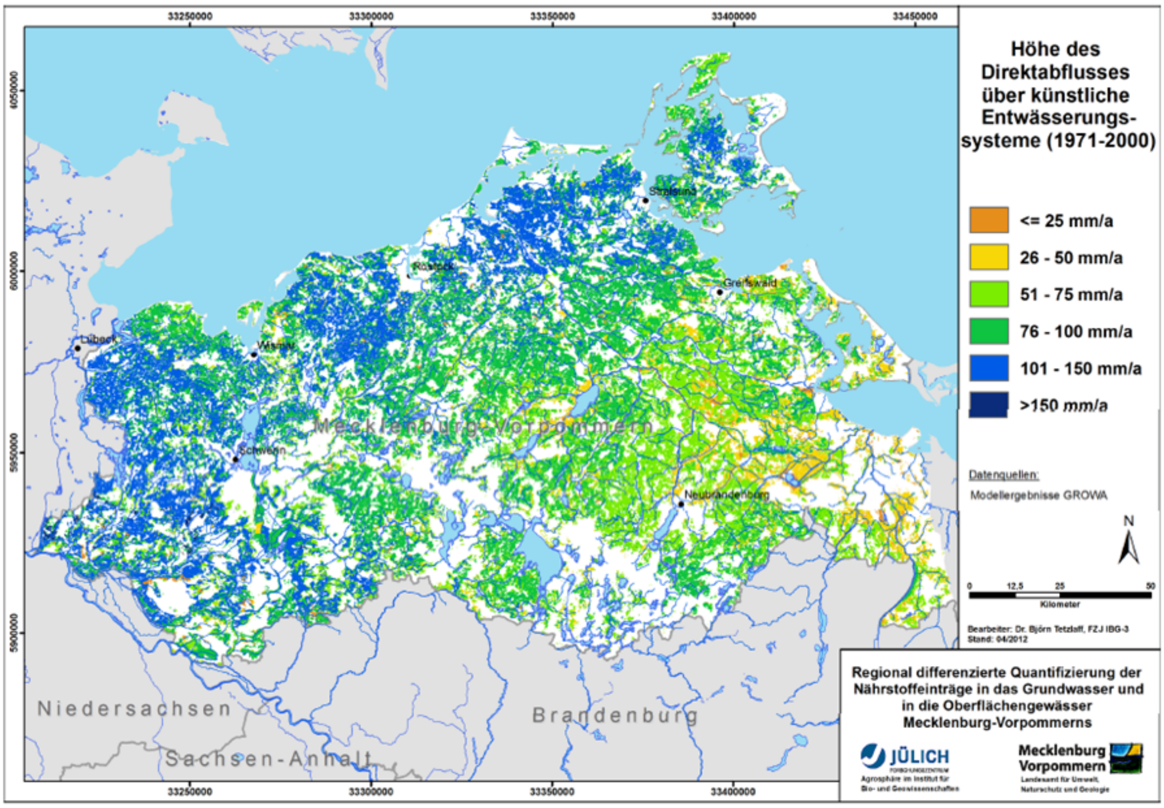
Drainage data were available for drained agricultural areas in some German federal states. It was decided to focus on potentially drained agricultural areas in Northern Germany, because drainage via tile drains is expected to be more important in the Northern German lowland, and relevant geodata were available to a higher extent in northern federal states.

Federal states (Bundesländer)	Abbre-viation	Spatial data for potentially drained areas	Drainage rate data for potentially drained areas	Drained agricultural area defined in GeoPELMO DE
Brandenburg	BB	available, not applicable*	not available*	yes
Lower Saxony	NI	available	available	yes
Mecklenburg-West Pomerania	MV	available	available	yes
North Rhine-Westphalia	NW	available	not available*	yes
Saxony	SN	available	not available*	yes
Saxony-Anhalt[15]	ST	available	available	yes
Schleswig-Holstein	SH	available	not available*	yes

* potentially drained areas and drainage rates were defined according to soil type classes based on drainage data from neighbouring federal states

In addition, drainage discharge was also quantified in projects in several federal states (e.g. Figure 36 for Mecklenburg-West Pomerania). Corresponding data was available from the three federal states of Lower Saxony, Mecklenburg-Western Pomerania and Saxony-Anhalt and was used for further analyses.

Figure 36: Calculated mean drainage discharge height (1971-2000) in Mecklenburg-West Pomerania



Source: Wendland et al. 2015, p. 109

4.5.2 Evaluation and definition of drained agricultural areas in Northern Germany

Because artificial drainage installations play a significant role in the northern lowland regions in Germany and most geodata was available here, it was decided during the project to develop a systematic approach to define potentially drained agricultural areas for GeoPELMO DE based on different soil types in seven federal states in Northern Germany: Schleswig-Holstein (SH), Mecklenburg-West Pomerania (MV), Brandenburg (BB), Saxony-Anhalt (ST), Saxony (SN), Lower Saxony (NI) and North Rhine-Westphalia (NW). Spatially differentiated data of potentially drained areas was available for six federal states. A descriptive statistical evaluation of the available data was performed to analyse the portion of potentially drained areas depending on different soil type classes from the general soil map BÜK250. For each occurring main soil type class, the percentage of the agricultural area was calculated. Furthermore, the percentage of the drained area within each soil type class was determined. The used soil classes are based on the official German soil survey guideline (BKA 5 2005):

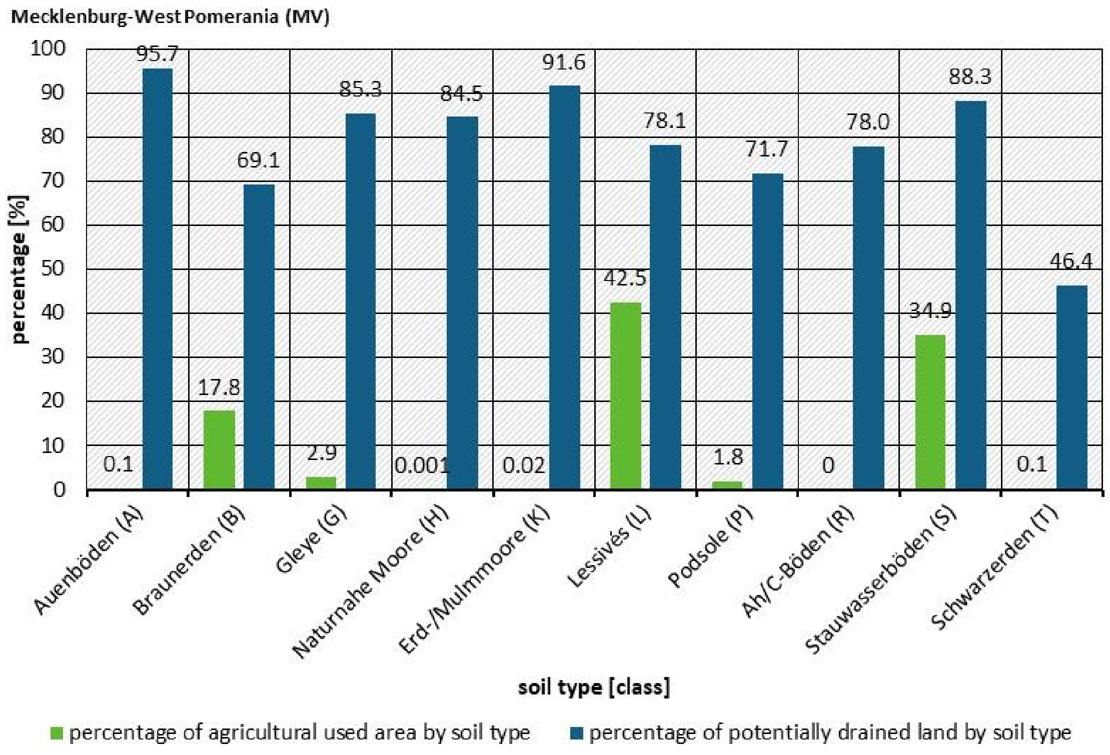
Soil types

The following soil classes and types according to the official German Soil Survey Guideline (BKA 5 2005) were used to determine the share of potentially drained areas in Northern Germany. The soils in brackets correspond to Reference Soil Groups of the IUSS Working Group WRB (2022):

A	Auenböden (Fluvisols)
B	Braunerden (Cambisols, Brunic Arenosols)
D	Pelosole (Vertisols, (Proto-)Vertic Cambisols)
G	Gleye (Gleysols)
H	Naturnahe Moore (Histosols)
K	Erd- und Mulmmoore (Histosols)
L	Lessivés (Luvisols, Alisols)
M	Marschen (Gleysols)
P	Podsole (Podzols)
R	Ah/C-Böden (Regosols, Phaeozems)
S	Stauwasserböden (Stagnosols, Planosols)
T	Schwarzerden (Phaeozems, Chernozems)
Y	Terrestrische anthropogene Böden (Anthrosols)

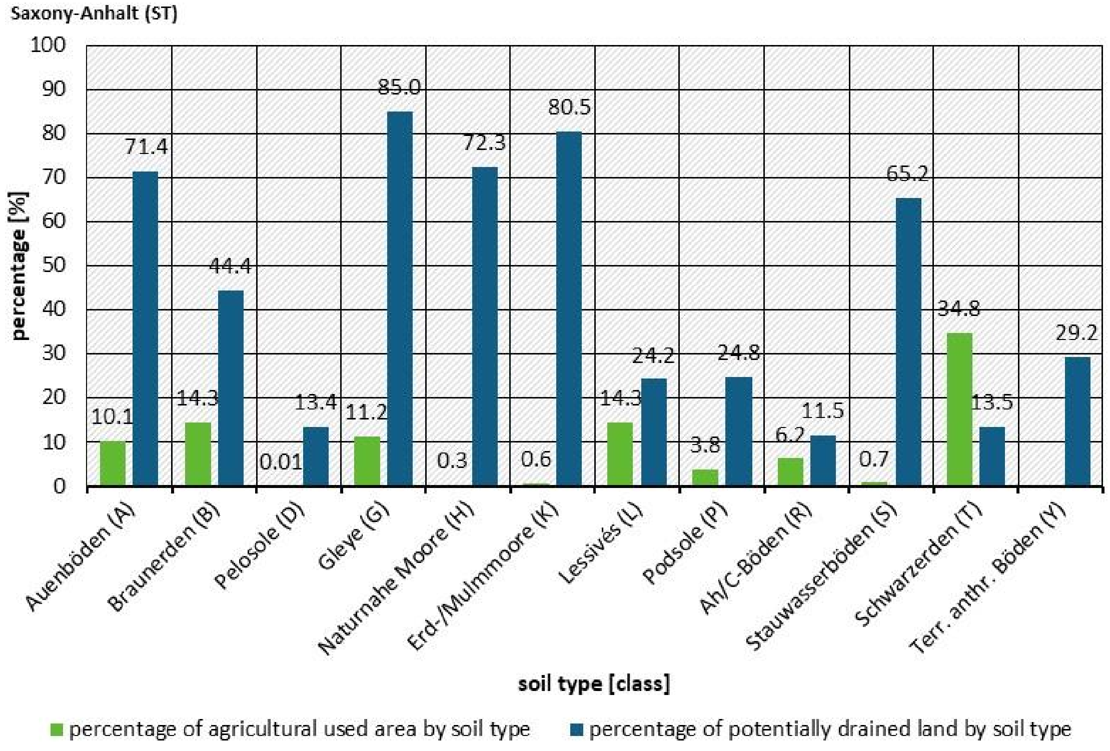
The following Figure 37 to Figure 43 show the percentage of different soil classes as ratio of total agricultural area in blue bars and the percentage of potentially drained soils for each soil type class in green bars. The statistical results were used afterwards to define soil types by expert judgement, which are potentially drained to a high degree. A median significantly higher than 50 % was used as main criterion. The outcome was used to define potentially drained areas in Brandenburg based on comparable soil type classes, because drainage data was not available. As the result, the soil type classes ´Auenböden´ (A: Fluvisols), ´Gleye´ (G: Gleysols), ´Naturnahe Moore´ (H: Histosols), ´Erd- und Mulmmoore´ (K: Histosols), ´Lessivés´ (L: Luvisols, Alisols), ´Marschen´ (M: Gleysols), ´Ah/C-Böden´ (S: Stagnosols, Planosols) were proposed to considered as completely drained in Brandenburg. However, some of those soil types like ´Naturnahe Moore´ (H: Histosols), ´Erd- und Mulmmoore´ (K: Histosols) and ´Marschen´ (M: Gleysols) do not or hardly ever occur in Brandenburg. (see Table 37).

Figure 37: **Percentage of potentially drained soil types in the agricultural area in Mecklenburg-West Pomerania**



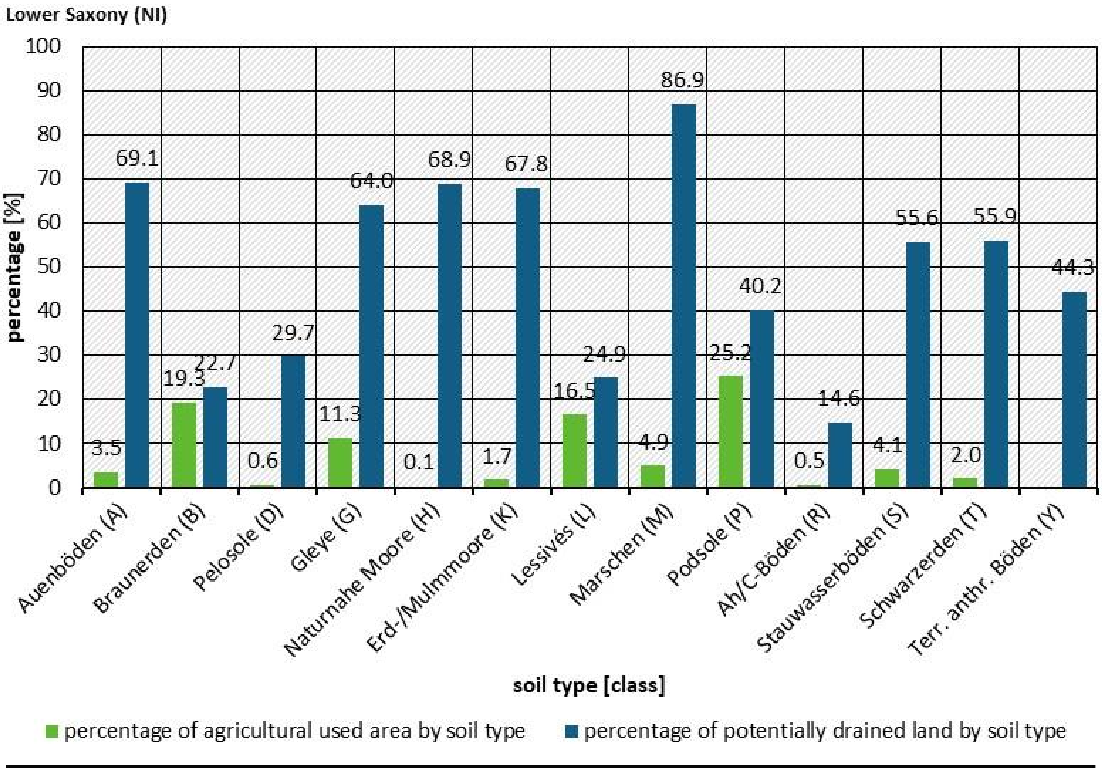
Source: own illustration, Fraunhofer IME.

Figure 38: **Percentage of potentially drained soil types in the agricultural area in Saxony-Anhalt**



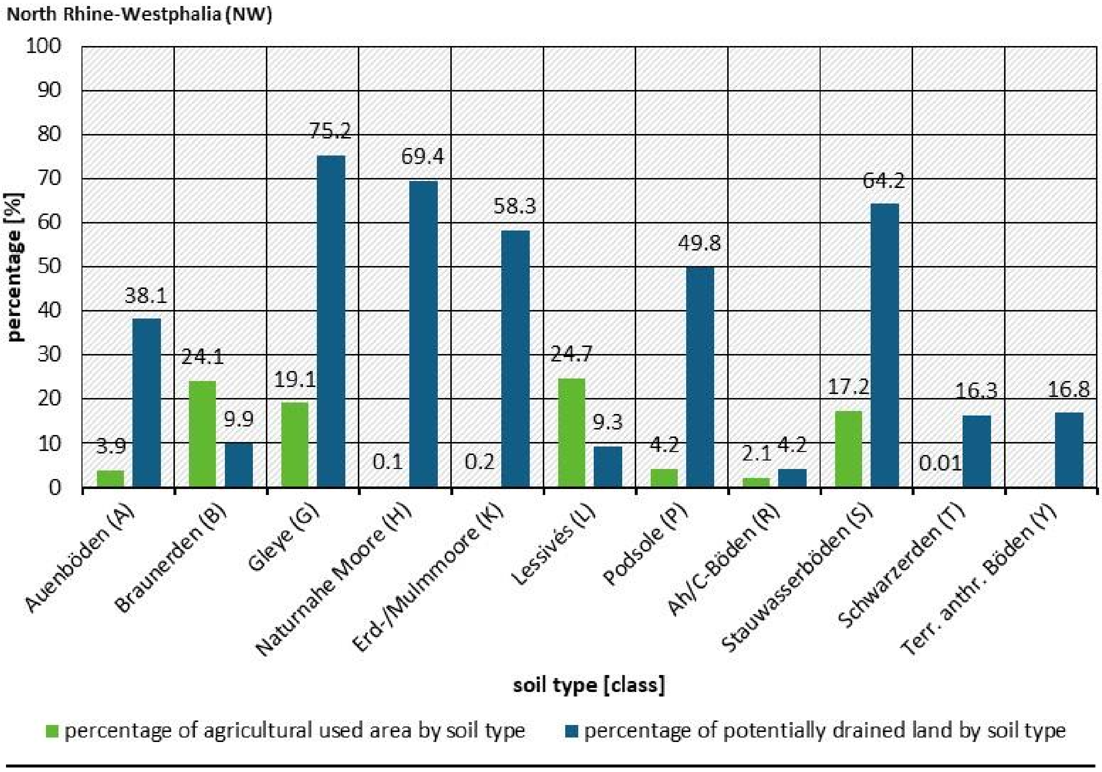
Source: own illustration, Fraunhofer IME.

Figure 39: Percentage of potentially drained soil types in the agricultural area in Lower Saxony



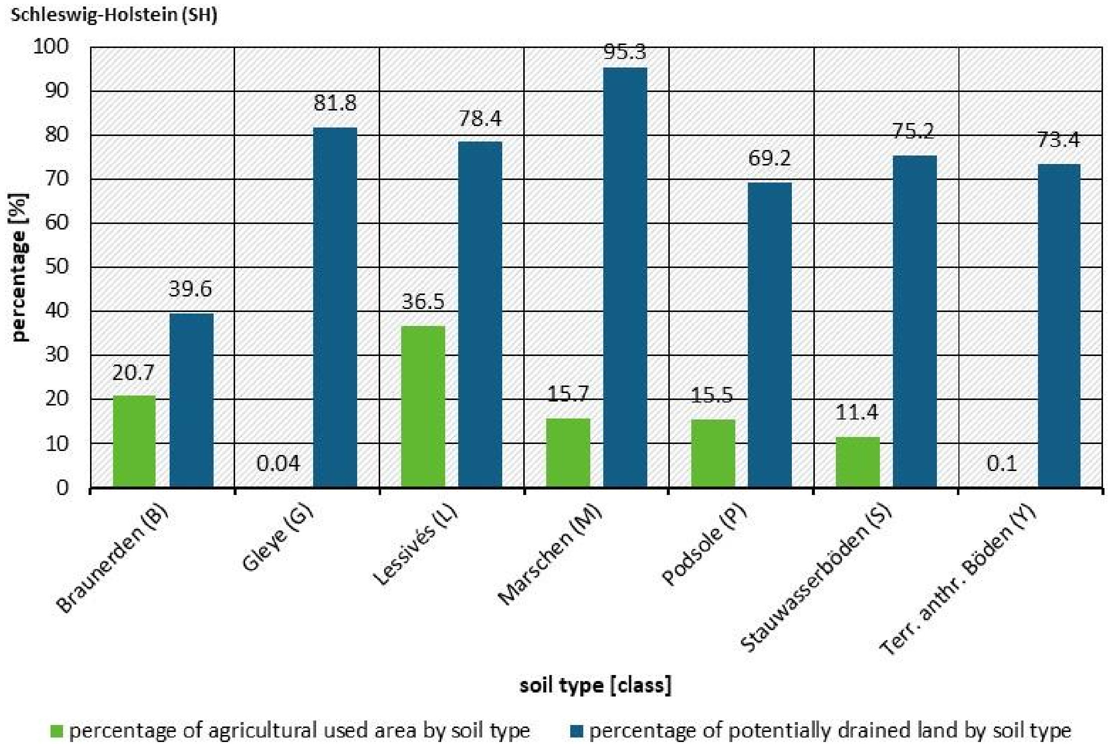
Source: own illustration, Fraunhofer IME.

Figure 40: Percentage of potentially drained soil types in the agricultural area in North Rhine-Westphalia



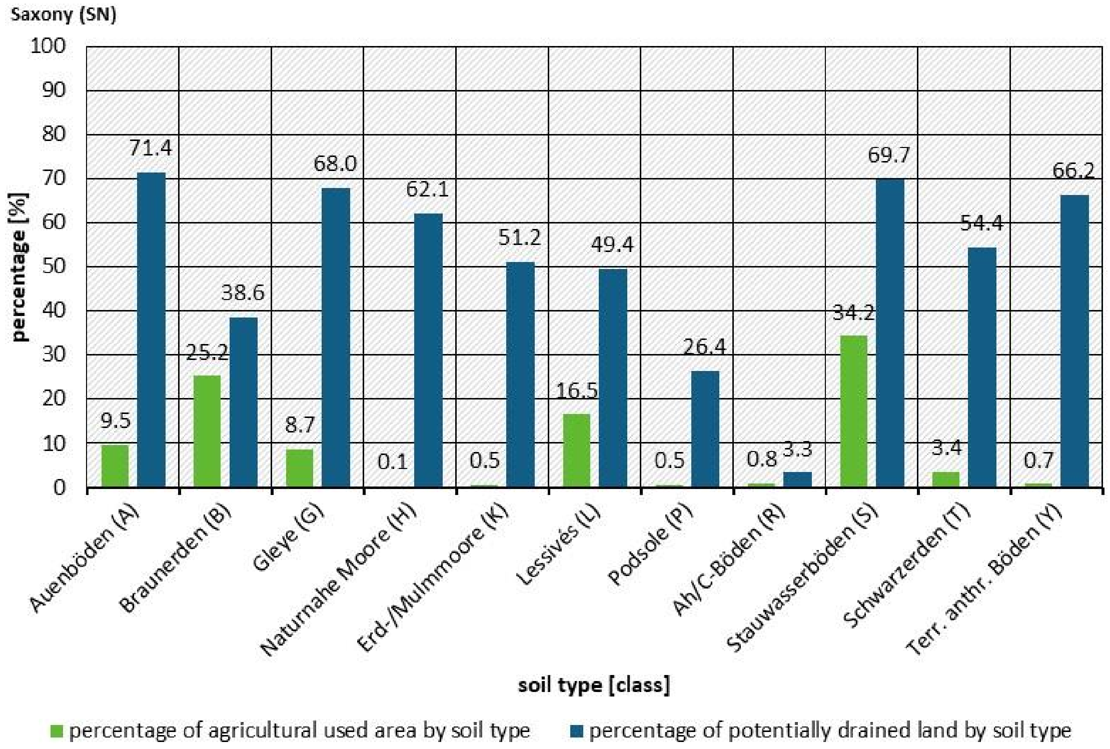
Source: own illustration, Fraunhofer IME.

Figure 41: Percentage of potentially drained soil types in the agricultural area in Schleswig-Holstein



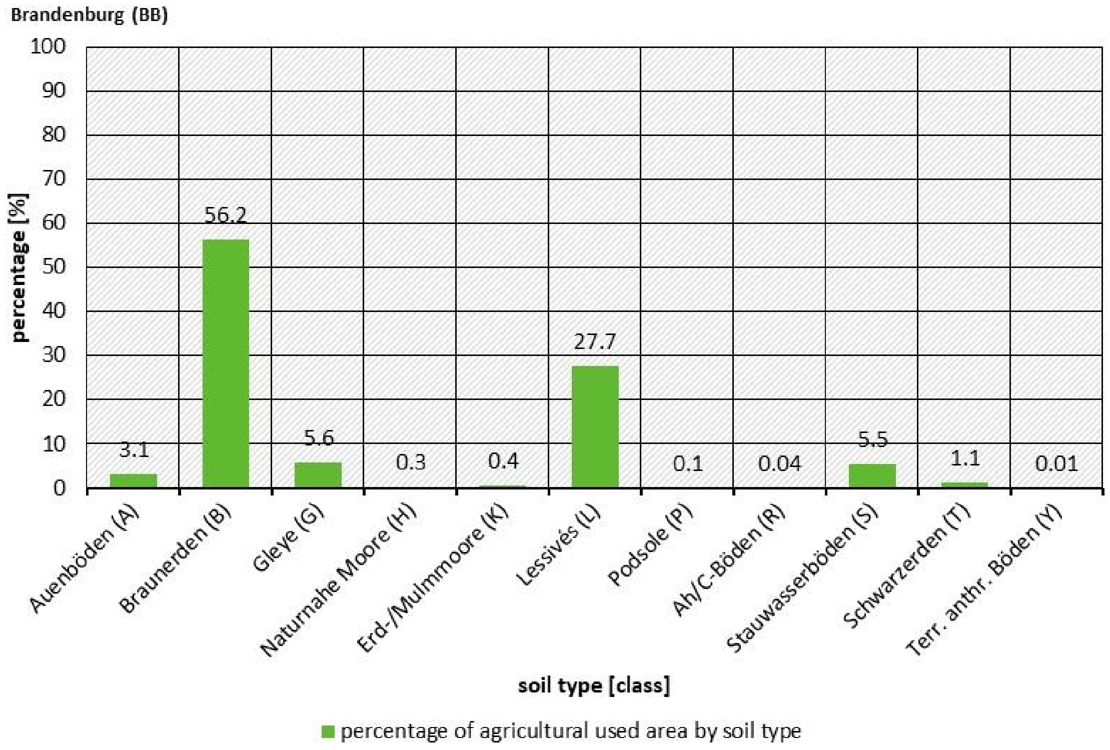
Source: own illustration, Fraunhofer IME.

Figure 42: Percentage of potentially drained soil types in the agricultural area in Saxony



Source: own illustration, Fraunhofer IME.

Figure 43: Percentage of soil types in the agricultural area in Brandenburg



Source: own illustration, Fraunhofer IME.

Table 37: Evaluation of potentially drained agricultural area in Northern Germany

A descriptive statistical evaluation of potentially drained agricultural areas in relation to soil type classes from BÜK250 (BGR 2018b) in Lower Saxony (NI), Mecklenburg-West Pomerania (MV), North Rhine-Westphalia (NW), Saxony-Anhalt (ST), Saxony (SN), Schleswig-Holstein (SH) was performed to define potentially drained soil types in Brandenburg (BB), where no drainage data were available.

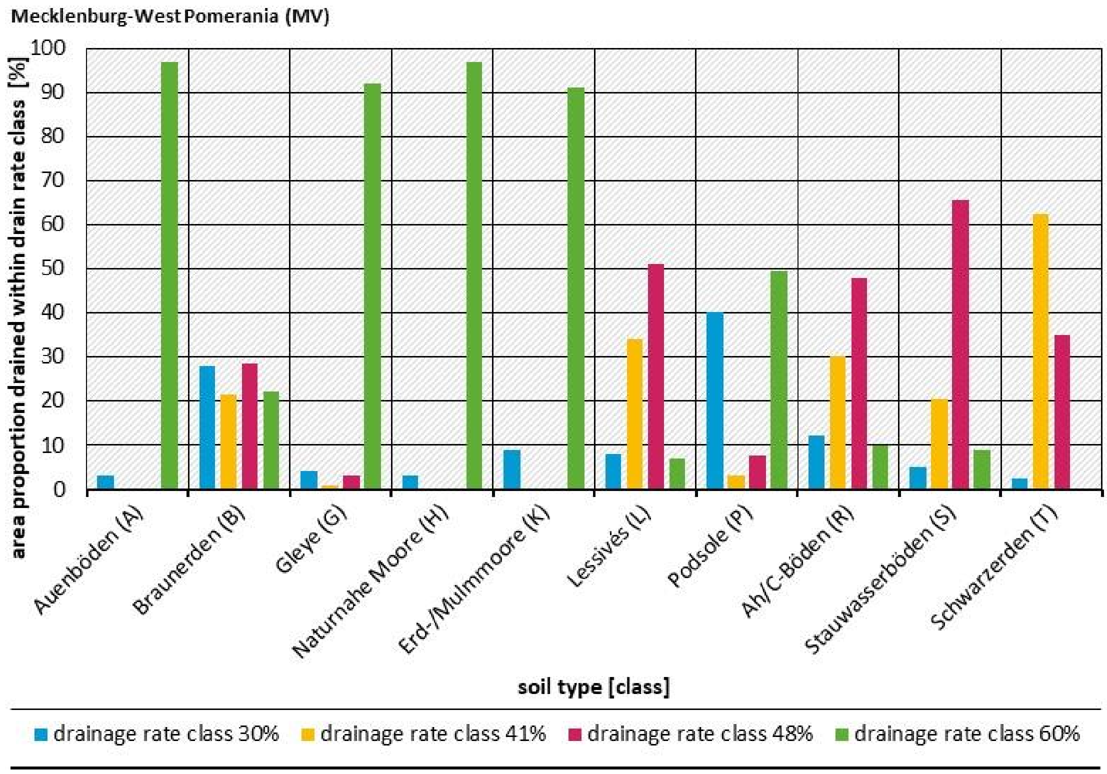
Soil type class*	Potentially drained soils per soil class in agricultural area [%]						Statistic of potentially drained soils per soil class in 5 federal states [%]					Defined as drained area in BB [%]	Occurrence of soil classes in agricultural area in BB [%]
	NI	MV	NW	ST	SN	SH	median	arith. mean	min	max	range		
A	69	96	38	71	71	-	71	69	38	96	58	yes	3.1
B	23	69	10	44	39	40	39	37	10	69	59	no	56.2
D	30	-	-	13	-	-	22	22	13	30	16	no	0
G	64	85	75	85	68	82	79	77	64	85	21	yes	5.6
H	69	85	69	72	62	-	69	71	62	85	22	yes	0.3
K	68	92	58	81	51	-	68	70	51	92	40	yes	0.4
L	25	78	9	24	49	78	37	44	9	78	69	yes	27.7
M	87	-	-	-	-	95	91	91	87	95	8	(yes)	0
P	40	72	50	25	26	69	45	47	25	72	47	no	0.05

Soil type class*	Potentially drained soils per soil class in agricultural area [%]						Statistic of potentially drained soils per soil class in 5 federal states [%]					Defined as drained area in BB [%]	Occurrence of soil classes in agricultural area in BB [%]
	NI	MV	NW	ST	SN	SH	median	arith. mean	min	max	range		
R	15	78	4	12	3	-	12	22	3	78	75	no	0.04
S	56	88	64	65	70	75	67	70	56	88	33	yes	5.5
T	56	46	16	14	51	-	46	37	14	56	42	no	1.1
Y	44	-	17	29	66	73	44	46	17	73	57	no	0.01

* see names for soil type classes in the frame above.

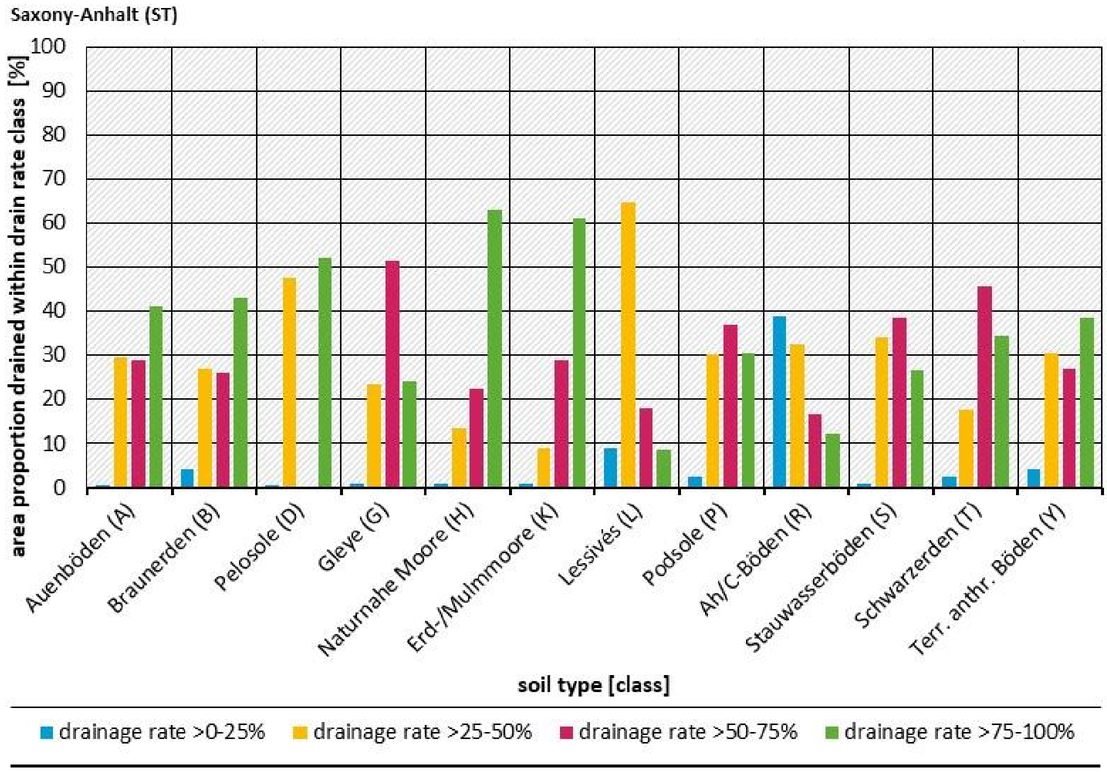
Information on the quantity of drainage fluxes was only available for potentially drained areas in the three federal states: Mecklenburg-West Pomerania (MV), Lower Saxony (NI) and Saxony-Anhalt (ST). In the next step, the drainage rates within the soil type classes from the soil map BÜK250 were calculated for each of those three federal states. The total amount of drained water is related to the total amount of leachate to obtain the percentage of drainage water (see Figure 44 for MV and Figure 45 for ST). It must be considered that drainage rate data for potentially drained areas was provided in different formats. In Mecklenburg-West Pomerania (MV) the proportion of drainage in relation to leachate amounts is specified in four classes between 30 % and 60 %. The four calculated drainage rates (Figure 44) indicate that the drainage data have been derived/calculated from fixed percentage of other water fluxes before.

Figure 44: Calculated proportion of drainage depending on the leachate rate in Mecklenburg-West Pomerania



Source: own illustration, Fraunhofer IME.

Figure 45: Calculated proportion of drainage depending on the leachate rate in Saxony-Anhalt

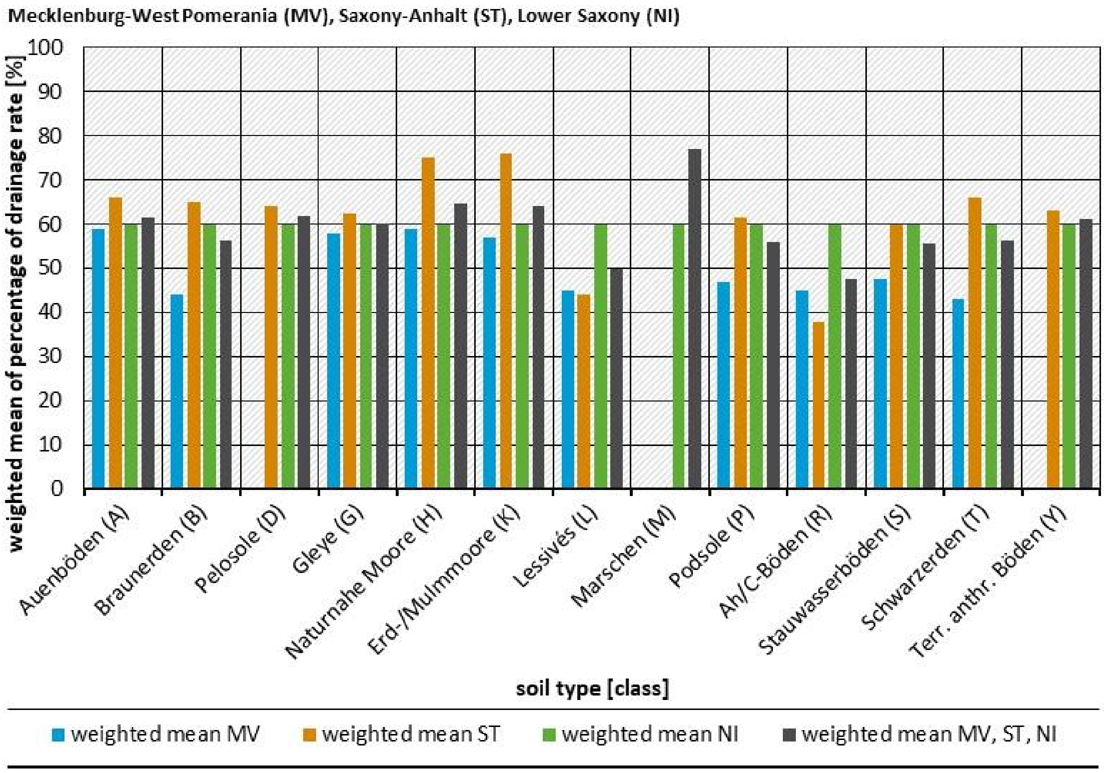


Source: own illustration, Fraunhofer IME.

For Lower Saxony, a uniform drainage rate of 60 % was calculated and provided for all potentially drained areas independent from the location or any soil type. In Saxony-Anhalt (ST), leachate and drainage data was provided from the modelling system ArcEGMO and continuous proportion values of drainage rates were available. Figure 45 shows the calculated drainage rates for each soil type class from the BÜK250 in four classes for better comparability.

This comparison shows that the determination of a reliable drainage rate for individual soil types is difficult and subject to uncertainties. There is no recognizable pattern, which is most likely due to the different data basis that was provided/used in the raw data. In order to obtain the most reliable data possible on the percentage of drainage rate per soil type class, another evaluation step became necessary. Based on the data in Mecklenburg-West Pomerania (MV), Lower Saxony (NI) and Saxony-Anhalt (ST), the total drained area per soil type and calculated percentage of drainage class was estimated. Subsequently, the weighted average was calculated for each soil type class. This resulted in a comparable drainage percentage for each soil type and federal state, which was then aggregated to one mean value per soil type. Figure 46 shows the resulting mean percentages of drainage values per soil class for each of the three federal states (coloured bares) and the overall mean proportion for all three states (grey bars). The overall mean percentages for all soil type classes (Table 38) were used to define drainage rates in all seven northern federal states: Schleswig-Holstein (SH), Mecklenburg-West Pomerania (MV), Brandenburg (BB), Saxony-Anhalt (ST), Saxony (SN), Lower Saxony (NI) and North Rhine-Westphalia (NW). These average values were assigned to the soil type classes and potentially drained areas in the six federal states Schleswig-Holstein (SH), Mecklenburg-West Pomerania (MV), Saxony-Anhalt (ST), Saxony (SN), Lower Saxony (NI) and North Rhine-Westphalia (NW). For this purpose, the potentially drained areas were intersected with the agricultural area and the soil type classes of the BÜK250. For Brandenburg, the calculated mean drainage rates were assigned to the entire agricultural area of the soil class types mentioned above due to absence of drainage data. Furthermore, additional data on the drainage rate for the soil type class 'M' in Schleswig-Holstein (SH) was available. This data was used to calculate an area-weighted average for this soil type class based on Schleswig-Holstein and Lower Saxony data, resulting in a drainage rate of 77 %. Figure 47 finally provides an overview about the areas assumed to be drained in GeoPELMO DE and the drainage rates for each soil type class.

Figure 46: Calculated drainage rates per soil type class (weighted mean)



Source: own illustration, Fraunhofer IME.

Table 38: Calculated mean percentages of drainage rates per soil type class from the German soil map BÜK250 according to BGR (2018b)

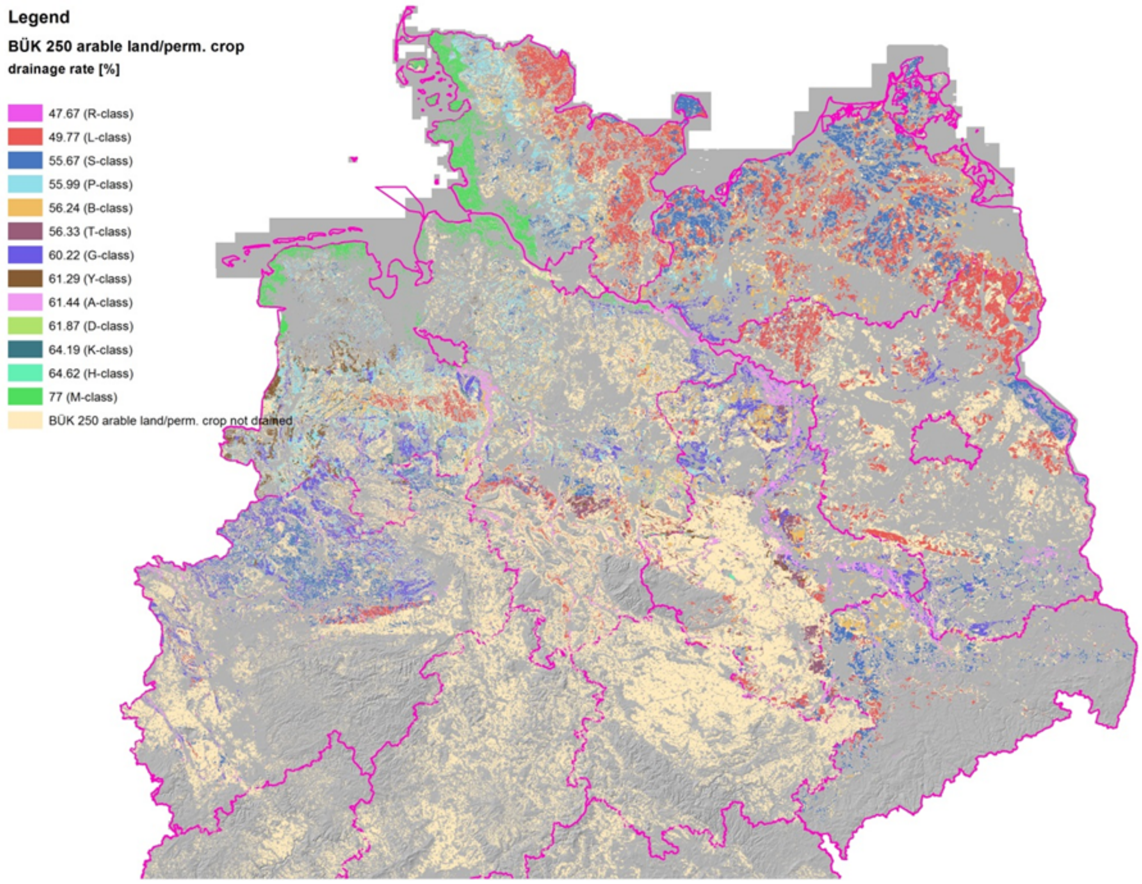
The percentage of drainage from leachate was calculated as mean value from drainage rate data available for Mecklenburg-West Pomerania, Lower Saxony and Schleswig-Holstein.

Soil type class [-]	Soil type name [-]	Drainage rate [%]
A	Auenböden (Fluvisols)	61.44
B	Braunerden (Cambisols, Brunic Arenosols)	56.24
D	Pelosole (Vertisols, (Proto-)Vertic Cambisols)	61.87
G	Gleye (Gleysols)	60.22
H	Naturnahe Moore (Histosols)	64.62
K	Erd- und Mulmmoore (Histosols)	64.19
L	Lessivés (Luvisols, Alisols)	49.77
M	Marschen (Gleysols)	77.0*

Soil type class [-]	Soil type name [-]	Drainage rate [%]
P	Podsole (Podzols)	55.99
R	Ah/C-Böden (Regosols, Phaeozems)	47.67
S	Stauwasserböden (Stagnosols, Planosols)	55.67
T	Schwarzerden (Phaeozems, Chernozems)	56.33
Y	Terrestrische anthropogene Böden (Anthrosols)	61.29

* The percentage was calculated as mean value from drainage rates in Lower Saxony and Schleswig-Holstein, only.

Figure 47: Map of agricultural drained areas in Northern Germany and drainage rates for all drained soil type classes



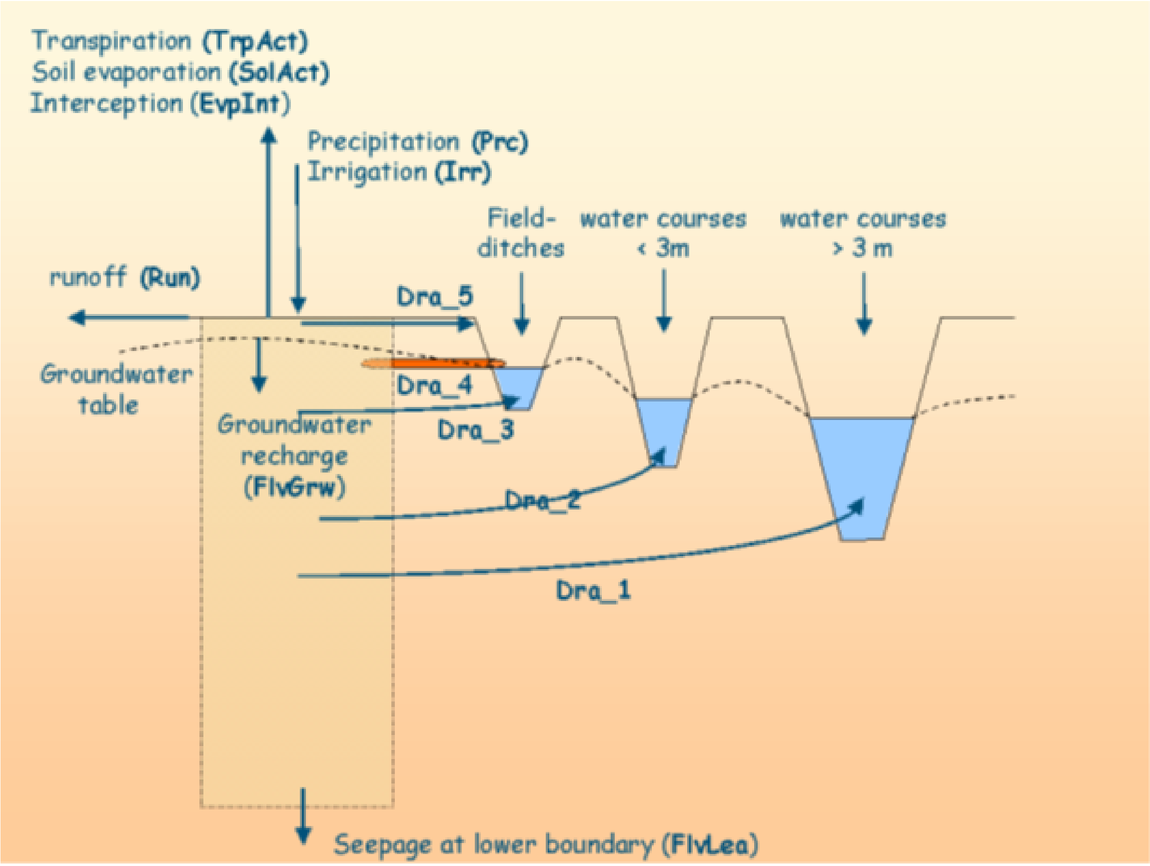
Source: own illustration, Fraunhofer IME.

4.5.3 Drainage in common leaching models PELMO and PEARL

The loss of percolate volumes due to drainage systems cannot be calculated with PELMO as the original PELMO is a one-dimensional model. In contrast, GeoPEARL-NL can calculate groundwater concentrations considering the effect of drainage systems (see Tiktak et al. 2003).

According to Tiktak et al. (2003) the Dutch model implementation shows that – if rapid drainage mechanisms (i.e. tube drainage and surface drainage) are dominating – the estimated transport of pesticides into local surface waters will be higher than the average fluxes of pesticide leaching into local groundwater aquifers. To simulate the effect of drainage systems the soil hydrology in PEARL was combined with a regional groundwater model. Results from this project allowed building a new spatially distributed pesticide leaching model for the Netherlands, which does distinguish between drainage fluxes and the flow to the regional groundwater. In GeoPEARL, different classes of local drainage systems into surface water courses can be considered (see Figure 48).

Figure 48: The GeoPEARL water balance



Source: Tiktak et al. 2003, p. 71

"The definition of these classes was inferred from 1:10,000 Dutch topographical maps. The fourth and fifth drainage systems were used for tube drainage and rapid discharge at the soil surface, respectively. Surface drainage occurs if the groundwater table is near the soil surface. The feature of defining the local drainage fluxes separately allows the calculation of residence times of pesticides in the saturated zone." (Tiktak et al., 2003, p. 20)

4.5.4 Technical concept to consider drainage in PELMO

4.5.4.1 Definition of a drainage factor and drainage depth in GeoPELMO DE

The soil inventory and soil hydrology in the Netherlands and in Northern Germany are comparable to a certain extent. Therefore, the consideration of drainage in a spatial distributed model like GeoPELMO DE would result in a more realistic evaluation of the soil water content for Germany. Because PELMO is a one-dimensional model and drainage is not considered yet as three-dimensional process, a new drainage model concept must be implemented to consider the effect of drainage for the estimation of soil water percolates. The following concept was developed during the project.

Dependent on the efficiency of the drainage system (factor f_{eff}) PELMO's standard percolate (P_{total}) is reduced to obtain the effective percolate amount below the assumed drainage system (= P_{eff}):

$$P_{eff} = \left(1 - f_{eff}\right) \cdot P_{total} \qquad (4)$$

The drainage efficiency factor should be set to 0, if there is no artificial drainage system. A factor of 1 means, that the total amount of percolate will be directed into the drainage system. This parameter should not be confused with the responses of the drainage system to precipitation. The drainage efficiency factor refers to the percolate amount that reaches the base of the drainage system.

The depth of the drainage system is required as a second parameter to correct the current percolate amounts in GeoPELMO DE considering the losses through the drainage. However, no spatial information is available on the depth of existing artificial drainage systems. For model implementation, it is therefore assumed that the drainpipes are always installed at a soil depth of 80 cm, i.e. 20 cm above the regulatory standard depth of 1 m.

4.5.4.2 Analysis of seasonal drainage effects in simulations with GeoPELMO DE

To compare drainage results calculated with PELMO with drainage response to precipitation on a field scale, a simulation was performed using the FOCUS Hamburg scenario and winter cereals. Two annual periods of the simulation were further analysed, which are characterised by normal (783 mm/a) and high (1028 mm/a) annual precipitation, respectively. The following two figures show the daily precipitation and the daily drainage responses at 80 cm soil depth, when an efficiency factor of 1 is used. That means that all percolate amounts are assumed to be directed into the artificial drainage system. Figure 49 shows an average situation. Relevant drainage amounts are simulated with PELMO in the spring and winter period, but no drainage fluxes are calculated in summer and autumn due to dry soil moisture conditions.

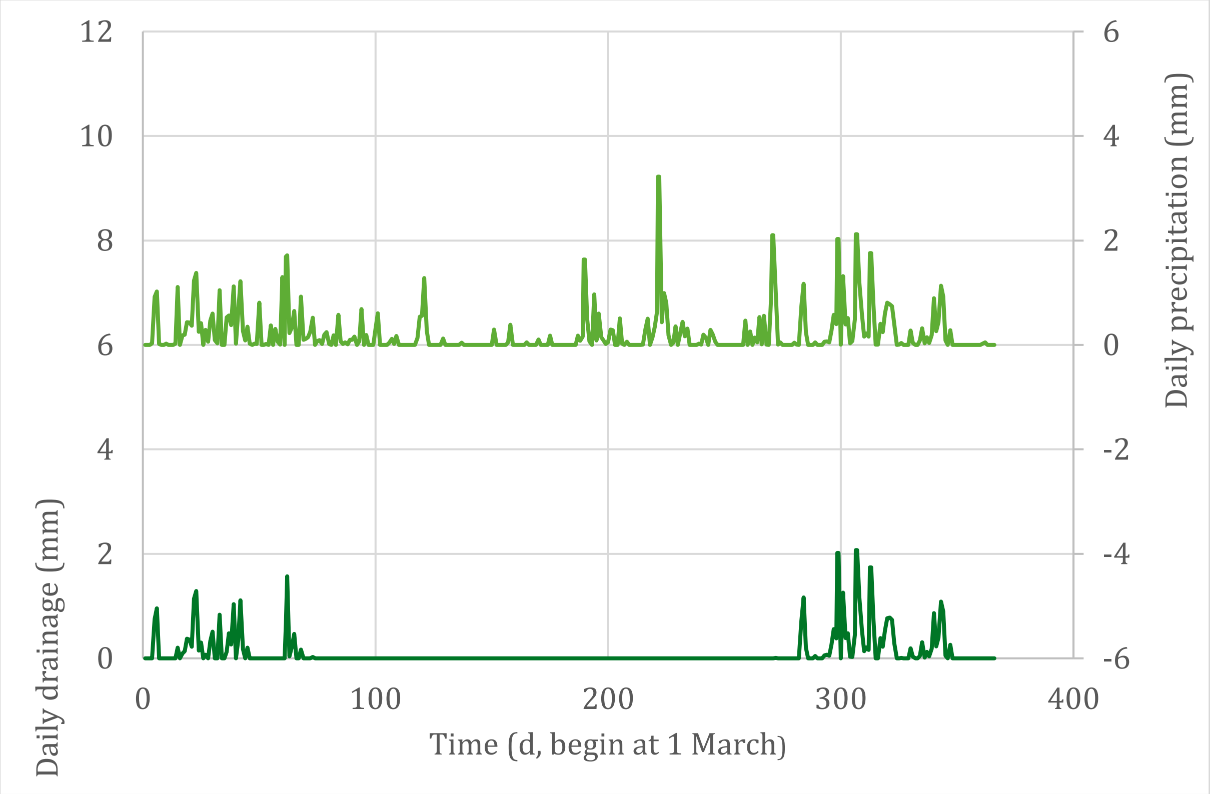
The drainage responses are always fast. In Table 39 the seasonal results are presented for two different drainage system efficiency factors 0.8 and 1.0. The drainage responses are provided as percentage of the precipitation. As already shown in Figure 49 PELMO did not simulate any drainage response for the summer and the autumn period. For the spring period the average drainage response was 29 % (f_{eff} = 1) and 23.2% (f_{eff}=0.8). However, dependent on the actual soil moisture content the drainage amounts cover a significant range as demonstrated by the 90th percentiles (response 86 % for f_{eff}=1 and 69 % for f_{eff}=0.8). Maximum drainage responses were found in the winter period with an average of 70 % and 56.2 % for f_{eff}=1 and f_{eff}=0.8, respectively.

Figure 50 shows the situation for an annual period with higher precipitation. Drainage flows are simulated with PELMO throughout the year with drainage flows generally lower in spring than in other seasons.

Same as in the annual period with normal precipitation the response of the drainage system is always fast. In the following table the seasonal results are presented for two different drainage system efficiency factors 0.8 and 1.0. The lower responses were simulated for the spring period with average percentages of 7.3 % (f_{eff} = 1) and 5.8 % (f_{eff}=0.8). For the same period also the 90th percentiles of drainage proportions were relatively low with 17 % and 13 %. Due to the high precipitation in summer the drainage fluxes were significantly higher than in spring with average amounts of 20 % (f_{eff}=1) and 16 % (f_{eff}=0.8). Maximum average drainage proportions up to 70 % (f_{eff}=1) were calculated for the winter period. The 90th percentiles of the drainage proportions in autumn and winter seasons were even higher with 98 % (autumn, f_{eff}=1) and 100 % (winter, f_{eff}=1).

Figure 49: **Precipitation and drainage response [mm] at 80 cm soil depth calculated with PELMO**

The FOCUS Hamburg scenario in combination with winter cereals is used in the simulation run. The annual precipitation for the FOCUS year is 783 mm/a. The drainage efficiency factor (*f_{eff}*) was set to 1.



Source: own illustration, Fraunhofer IME.

Table 39: **Daily drainage percentages [%] related to precipitation for two different drainage efficiency factors calculated with PELMO**

For the simulation run the FOCUS Hamburg scenario in combination with winter cereals was used. The FOCUS weather years 15/16 were selected for the analysis, which represent a period with normal precipitation.

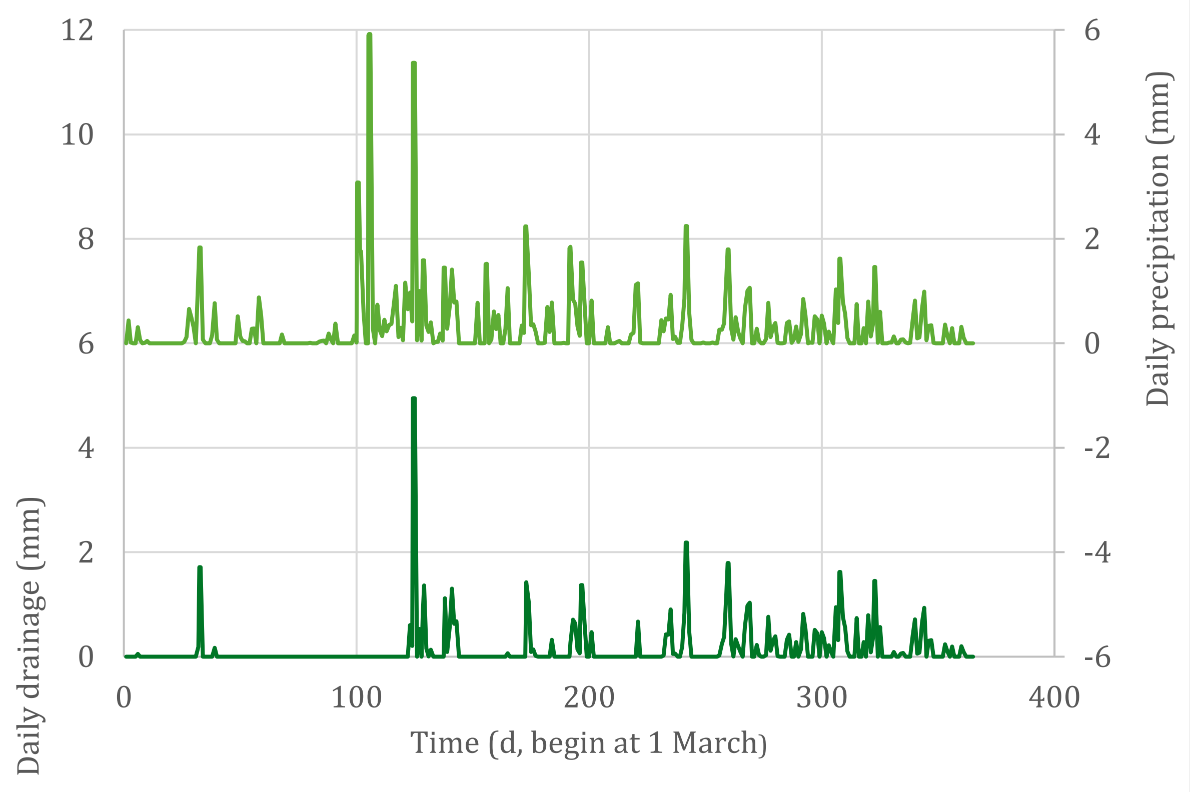
Drainage efficiency f_{eff}	**1.0**	**1.0**	**0.8**	**0.8**
Statistical parameter	**Arithmetic mean**	**90th percentile**	**Arithmetic mean**	**90th percentile**
Spring	29.0	86.0	23.2	68.8
Summer	0	0.0	0.0	0.0
Autumn	0	0.0	0.0	0.0
Winter	70.2	99.6	56.2	79.7
Year	**31.3**	**96.8**	**25.0**	**77.4**

The previous analysis was based on daily responses of the drainage system in PELMO to precipitation amounts. To compare the results with experimental findings, the seasonal precipitation and drainage/percolate amounts were calculated for the whole FOCUS weather period of 20 years in the FOCUS Hamburg scenario. The results are summarised in the following

Table 41. The differences between the results in Table 39/Table 40 and Table 41are caused by the different aggregation procedure (daily versus seasonal data).

Figure 50: Precipitation and drainage response [mm] at 80 cm soil depth calculated by PELMO

The FOCUS Hamburg scenario in combination with winter cereals was used in the simulation run. The annual precipitation for the FUCUS year is 1028 mm/a. The drainage efficiency factor (f_{eff}) was set to 1.



Source: own illustration, Fraunhofer IME

Table 40: Daily drainage percentages [%] related to precipitation for two different drainage efficiency factors calculated with PELMO

For the simulation run the FOCUS Hamburg scenario in combination with winter cereals was used. The FOCUS weather years 12/13 were selected for the analysis, which represent a period with high precipitation.

Drainage efficiency f_{eff} **Statistical parameter**	**1.0** **Arithmetic mean**	**1.0** **90th percentile**	**0.8** **Arithmetic mean**	**0.8** **90th percentile**
Spring	7.3	16.7	5.8	13.4
Summer	19.8	81.1	15.8	64.9
Autumn	49.2	97.7	39.3	78.1
Winter	70.3	99.9	56.2	79.9
Year	**39.5**	**97.9**	**31.6**	**78.3**

Table 41: Seasonal drainage response to precipitation over 20 years calculated by PELMO

For the simulation run, the FOCUS Hamburg scenario was selected in combination with winter cereals. The maximum drainage efficiency factor was used (f_{eff}=1.0).

FOCUS year [-]	Spring [%]	Summer [%]	Autumn [%]	Winter [%]	Year [%]
1	55.42	0.00	42.74	86.73	44.55
2	30.11	0.00	0.00	71.19	29.66
3	0.00	0.00	0.00	59.11	22.52
4	35.46	0.00	27.89	82.77	30.83
5	47.53	0.00	37.87	87.49	37.61
6	24.33	0.00	7.95	92.21	33.45
7	17.62	28.14	70.88	90.88	50.30
8	43.98	0.00	55.58	91.43	42.15
9	19.64	0.00	1.43	89.46	32.14
10	51.10	0.00	0.00	93.95	46.51
11	3.74	0.00	42.37	85.73	28.61
12	31.92	0.00	16.35	88.51	30.00
13	21.21	0.00	0.00	82.49	28.77
14	4.16	0.00	52.79	85.16	37.79
15	49.94	0.00	0.00	73.23	27.62
16	40.84	0.00	0.00	66.97	26.27
17	12.89	0.00	0.00	64.99	20.31
18	16.39	0.00	38.91	78.45	29.61
19	43.47	0.00	27.76	85.97	40.11
20	0.00	4.75	68.33	89.49	44.61
10th percentile	3.37	0.00	0.00	66.77	25.90
Median	27.22	0.00	22.05	85.85	31.48
90th percentile	50.06	0.48	56.86	91.51	44.80

The results show that the seasonal drainage responses to precipitation calculated by PELMO are characterised by high variability due to dependencies on soil moisture and precipitation patterns. This is in line with experimental data, where similar variations were observed. Depending on the rainfall intensity, experimental drainage values were in the range of 50 % to 100 % in autumn and winter and 40 % to 70 % in spring and summer (Hirt et al. 2011). Same as with the calculations, the measured values in the warm seasons also showed a stronger dependence on the precipitation intensity. It can be concluded from the comparison that the modelling results of PELMO do not contradict the results from field investigations with drainage systems.

However, the modelling results were only based on a single scenario typical for weather conditions in Northern Germany (FOCUS Hamburg). Therefore, additional simulations were performed with all soil-climate-combinations (n > 12000) using BÜK250 profiles and the corresponding climate scenarios, which are planned for the new version of GeoPELMO DE. Although drainage systems are only implemented in parts of these soil-climate-combinations, the simulations should nevertheless provide a broad overview of the percolate water at 80 cm soil depth in response to precipitation. The results are presented in the following table. For each soil-climate-combination the average seasonal response of the percolate flux at 80 cm soil depth to precipitation over a period of 20 years was calculated. The statistics represent the spatial variation (differences between the soil-climate-combinations) of the long-term average seasonal responses. As these are percolate fluxes, they should be compared with a maximum drainage efficiency (f_{eff}=1). Although not directly comparable, Table 7 5 confirms the seasonal effects of drainage fluxes from modelling compared with experimental findings (Hirt et al. 2011). The parameter drainage efficiency (f_{eff}) will be therefore implemented in the new version of GeoPELMO DE.

Table 42: Average seasonal percolate responses to precipitation calculated by PELMO

The statistical parameters represent different spatial percentiles of percolate percentages calculated in relation to seasonal precipitations. As reference crop winter cereals was used.

Season	10th percentile [%]	Median [%]	90th percentile [%]
Spring	14.5	25.0	38.1
Summer	0.9	4.9	15.3
Autumn	14.9	35.5	54.5
Winter	54.3	75.4	85.3
Year	21.2	30.2	48.3

4.5.4.3 Comparison of modelled drainage fluxes with drainage fluxes determined at Estrup

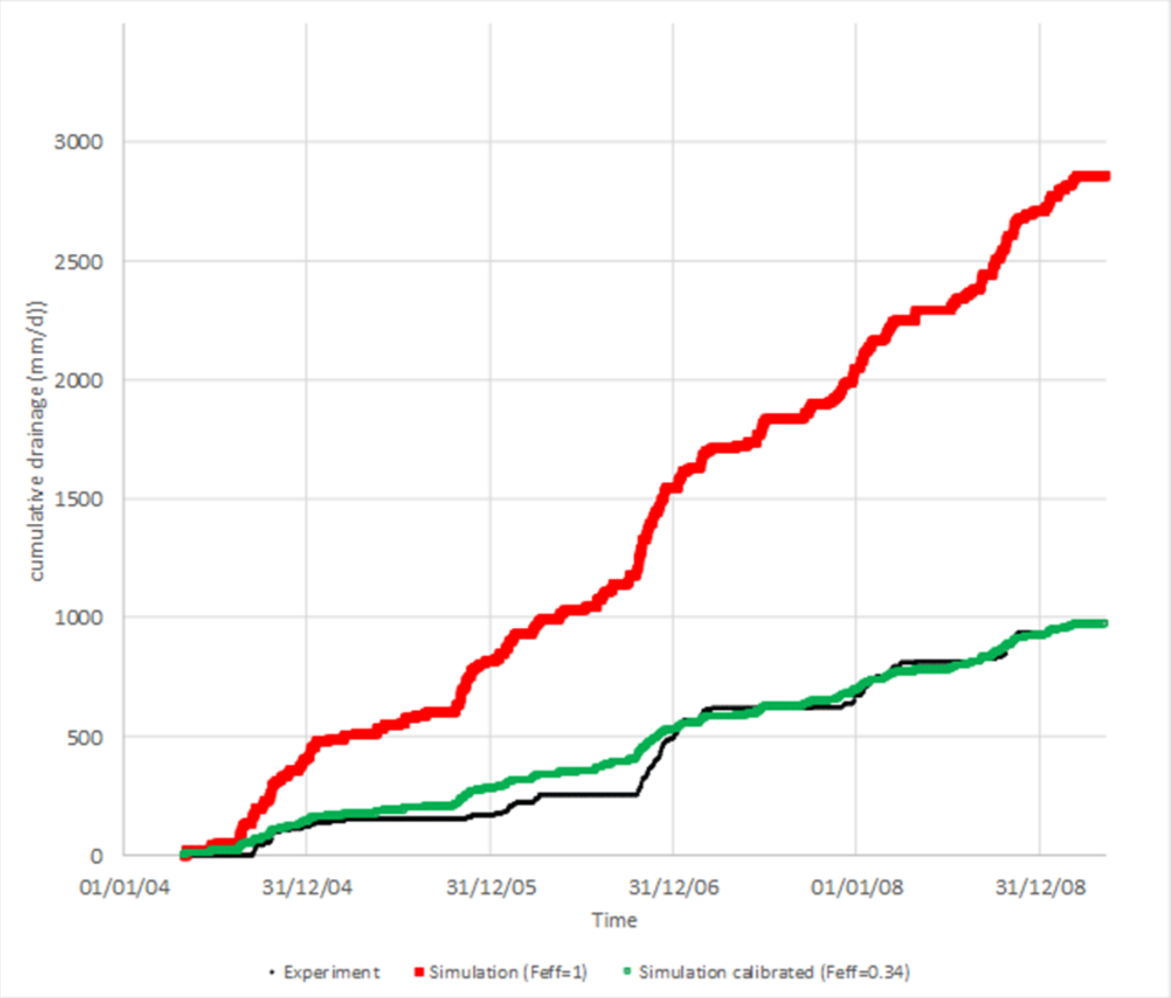
To verify the results of PELMO using more detailed experimental data, drainage discharges measured at the Estrup monitoring site were used. Daily drainage volumes were available for the time 01 May 2004 to 03 Jun 2009. Corresponding site-specific soil and climate data were used in the calculation.

The results are presented in Figure 51. The measured drainage discharge is shown cumulative as thin black line. The total percolate calculated by PELMO at 80 cm is shown as a thick red line. This corresponds to a drainage situation in which it is assumed that the entire percolate would be directed into the drainage system (f_{eff}=1). This is of course not a realistic reflection of the situation at the Estrup field. It is recognisable that the two curves diverge widely. After considering a drainage efficiency (f_{eff}) of 0.34, which was determined by simple calibration, the total drainage is massively reduced (green line in Figure 51). The measured and calculated drainage values fit rather well for most of the period and the cumulative curves are now much closer together. However, a general discrepancy between simulation and experiment can be recognised regarding drainage volumes in summer and winter: although PELMO simulated less drainage in summer than in winter, the experimental differences between the seasons in the test field are more distinct, especially in the first part of the simulation. Overall, less drainage discharge is measured in summer month and more in the winter months. This discrepancy is likely because drainage flows are primarily influenced by fluctuating groundwater levels. The one-dimensional leaching model PELMO does not currently account for groundwater levels. Instead, drainage flows are estimated based solely on the amount of percolating water at a specified depth in the unsaturated soil zone.

There is no simple way to improve the modelling routine in PELMO without complex calibration of input parameters, because the estimation of drainage fluxes is related to the calculation of soil hydrology in combination with fluctuation groundwater levels. This would for example include sensitive parameters like 'the minimum depth for evaporation' or the seasonal and crop dependent Kc-factors which control the amount of daily evapotranspiration from the soil profile.

Nevertheless, the decision was made to introduce a simple factor like the drainage efficiency (f_{eff}) for calculating drainage flows in the one-dimensional model GeoPELMO DE.

Figure 51: Experimental drainage responses between 01 May 2004 and 30 Jun 2009 at the Danish monitoring site Estrup compared to percolate volumes at 80 cm calculated by PELMO



Source: own illustration, Fraunhofer IME

4.5.5 Implementation of drainage in GeoPELMO DE

The decision was finally made to consider drainage in GeoPELMO DE to estimate more realistic leachate amounts for agricultural situations with artificial drainpipes.

Information from available drainage maps is used to define potentially drained agricultural areas in GeoPELMO DE for seven federal states in Northern Germany (chapter 4.5.1 and 4.5.2). A transfer of information was carried out based on defined soil type classes for Brandenburg. A scenario definition was technically realised by overlapping potential drainage maps from the federal states and the nationwide soil map BÜK250. Therefore, the number of geometries increased compared to the scenario definition without considering drained areas in GeoPELMO DE.

A simple drainage efficiency factor (f_{eff}) was developed and evaluated to calculate drainage fluxes based on percolate amounts from the unsaturated soil zone with the one-dimensional model PELMO (chapter 4.5.4). It is the intention to consider this factor only for artificial drainage water systems on agricultural fields. Further water losses due to (natural) hypodermic fluxes are explicitly not covered with this approach. Mean drainage rates were finally obtained for several soil type classes from the BÜK250. Corresponding spatial data have been made available from three federal states in Northern Germany (chapter 4.5.2). The different calculated drainage rates are used as spatially distributed drainage efficiency factors (f_{eff}) for all drained scenarios/geometries in GeoPELMO DE.

A standard soil depth of 80 cm was defined in PELMO to calculate the loss of drainage fluxes (f_{eff}) based on percolate amounts. This definition was necessary since no spatial information is available about the depth of existing artificial drainage systems in Northern Germany. The theoretical assumption behind is that drainpipes are always installed at a soil depth above the most often measured groundwater level. The leachate concentration in 1 m of soil depth is used as regulatory value and serves as a measure of groundwater contamination. Therefore, a corresponding smaller depth of 80 cm, which is 20 cm above the regulatory value, was selected. However, it is important to note that the depth of drains in reality may vary.

It can be expected that the new drainage routine in GeoPELMO DE will result in reduced water fluxes below 80 cm in drained agricultural fields. That will influence the residence time of water and pesticides below 80 cm, the residence time will finally increase. As there is more time for degradation in the top metre less pesticide fluxes will finally reach deeper soil layers below 80 cm. That will finally result in lower calculated percolate concentrations at the bottom of the soil core.

4.6 Technical adjustments and scenario definition in PELMO

Various geodata had to be overlapped to define nationwide scenarios in GeoPELMO DE in order to generate all possible combinations of climate conditions (i.e., daily weather data from the representative weather station) and soil profile characteristics for agricultural areas including macropore and runoff classification as well as potential drainage. The outcome of this GIS analysis led to 12,710 different soil-climate-combinations for Germany.

Polygons which represent very small agricultural areas below 2 km^2 were finally merged with polygons of higher areal representativeness to reduce the necessary CPU time for PELMO simulation runs. The procedure was to search for alternative polygons with the same soil and a weather station with very similar conditions. If no such combination was found, the corresponding polygon was not merged. After applying this procedure 7,481 soil-climate-combinations remained, which were used for the simulations with GeoPELMO DE.

To reduce the required CPU time even further the software was programmed in a way that four simulations can be performed in parallel, utilising various existing multiprocessor cores.

In addition, considerable extensions of the programming code became necessary to enable PELMO to read the different scenario combinations line by line, run the respective simulation and write the simulation results (e.g. the 80th percentile of annual concentrations in the percolate) to a file. This output file is the basis for all percolate maps as well as for additional tabular outputs.

To read the soil profile information from the BÜK250 into PELMO, a special table was created that contains all important soil information. This table replaces the previous standard, in which a separate file was created for each scenario. New code was programmed to enable PELMO to read this information and to load the profile information into the existing software for a simulation. To make PELMO runs more user-friendly internal loops were added that perform all simulations in a single batch. It is therefore not necessary for users to select individual scenarios before simulations are started.

With these modifications and extensions PELMO is principally able to perform nationwide leaching simulations for Germany in overall 12,710 scenarios. However, an additional interface had to be defined and programmed to functions as a link between PELMO and the post-processing routines that prepare the important output of a GeoPELMO DE run. The link was created based on a simple list in ASCII format, which contains the following information in each line:

- Polygon code (no)
- Soil profile code
- Drainage code (= 0/1 for yes/no)
- Weather station code

5 Spatially distributed modelling results with GeoPELMO DE

5.1 Substance properties and crops considered for the analysis

The spatial modelling results using GeoPELMO DE depend on pesticide properties and application pattern. To cover a reasonable range of situations three different fictive parent compounds and two different fictive transformation products were considered in the analysis. Different sorption constants (K_{foc}, 1/n), degradation rates in soil ($DegT_{50}$) and formation fractions (ff) were defined as main properties driving the leaching in the unsaturated soil zone (see following frame).

All simulations were performed in maize and winter cereals over a period of 26 years including a warming up period of 6 years and with annual applications one day before emergence of the crop. The application rate was in general 200 g/ha.

Fictive active substances and metabolites defined for modelling

Three different fictive parent compounds (P = active substances) and two fictive transformation products (M = metabolites) with different sorption and degradation values were defined:

P1 - mobile & fast degrading:	K_{foc}: 30 L/kg,	1/n: 0.9,	$DegT_{50}$: 10 d
P2 - moderately mobile & fast degrading:	K_{foc}: 60 L/kg,	1/n: 0.9,	$DegT_{50}$: 20 d
P3 - hardly mobile & rather persistent:	K_{foc}: 240 L/kg,	1/n: 0.9,	$DegT_{50}$: 80 d
M1 - very mobile & moderately persistent:	K_{foc}: 10 L/kg,	1/n: 0.9,	$DegT_{50}$: 40 d
M2 - mobile & rather persistent:	K_{foc}: 30 L/kg,	1/n: 0.9,	$DegT_{50}$: 80 d

Three different combinations of parent compounds and metabolites were considered for further modelling analysis:

P1 forms M2 with 100 % formation (ff: 1.0)

P2 forms M1 with 50 % formation (ff: 0.5) and parallel M2 with 50 % formation (ff: 0.5)

P3 forms M2 with 100 % formation (ff: 1.0)

5.2 Procedure to analyse sensitivity of additional processes in GeoPELMO DE

Compared to the standard FOCUS leaching modelling approach in PELMO and PEARL the additional processes runoff after heavy rainfall events, macropore flow and drainage were activated in simulations with GeoPELMO DE. To analyse the influence of these processes for different regions in Germany, different simulation runs were performed with GeoPELMO DE and the special processes were switched on one after the other. The evaluation of results is provided in a sequence of five simulation runs starting with the FOCUS standard approach on chromatographic flow and ending with simulations considering all special processes. The details of the sequence are provided in the following:

1. **FOCUS L: GeoPELMO DE simulations without additional processes:**

In these simulations only leaching by chromatographic flow in soil is considered which is used as standard for regulatory decision making in the EU using FOCUS models and FOCUS scenarios.

2. **FOCUS L+R: GeoPELMO DE simulations considering runoff:**

In this simulation the process runoff is considered. The aim of this simulation run is to locate the areas where runoff may be in principle important and to analyse its influence on nationwide estimated pesticide groundwater concentrations.

3. **FOCUS L+R+M: GeoPELMO DE simulations considering runoff and macropore flow:**

In these simulations the process macropore flow is additionally considered beside runoff. A fixed macropore length of 80 cm is used in GeoPELMO DE. Soils classified as 'high macropore flow' (12.3 % of agricultural area) are parametrised considering a minimum of static macropore flow of 4 % and a dynamic maximum of macropore flow of 8 % depending of the weather conditions. Soils classified as 'moderate macropore flow' (52.9 %) are parametrised considering 2 % as minimum for the static macropore flow fraction and 4 % as maximum for the dynamic macropore flow fraction. No macropore flow is considered for the remaining 34.8 % of the agricultural soils in Germany. The aim of this simulation run is to locate the areas where preferential may be in principle important and to analyse its influence on nationwide estimated pesticide groundwater concentrations.

4. **FOCUS L+R+M+D: GeoPELMO DE simulations considering runoff, macropore flow and drainage:**

In these simulations, artificial drainage at 80 cm soil depth is additionally considered beside runoff and macropore flow. Pesticide fluxes are temporarily removed out of the soil core by horizontal drainage flow. Therefore, the percolate volume below 80 cm is mainly reduced, which may lead to a reduction of the concentration at 1 m soil depth, because the travel time from 80 cm to 100 cm can be increased which gives more time for degradation. The aim of this simulation run is to locate the areas where drainage may be important and to analyse its influence on nationwide pesticide groundwater concentrations.

5. **FOCUS L+R+M+D*: GeoPELMO DE simulations considering different organic carbon contents for the organic matter class h0:**

The organic carbon class (which is strongly correlated with organic matter) is probably the most important factor to model leaching of a substance in soil depending on its mobility (K_{foc} value). In the soil profiles of the BÜK250, several deeper soil horizons are classified as h0. To check the sensitivity of the organic matter content for class h0 a variation is performed with 0.2 % organic carbon as default value for humus class h0 in all profiles independent on the soil depth. These simulations are preformed including all additional processes: runoff, macropore flow and drainage. Consequently, the respective results will be compared with step 4 in this sequence, where default organic carbon contents of 0.1 % and 0.2 % dependent on the soil depth are used for humus class h0.

5.3 Results for the soil water regime

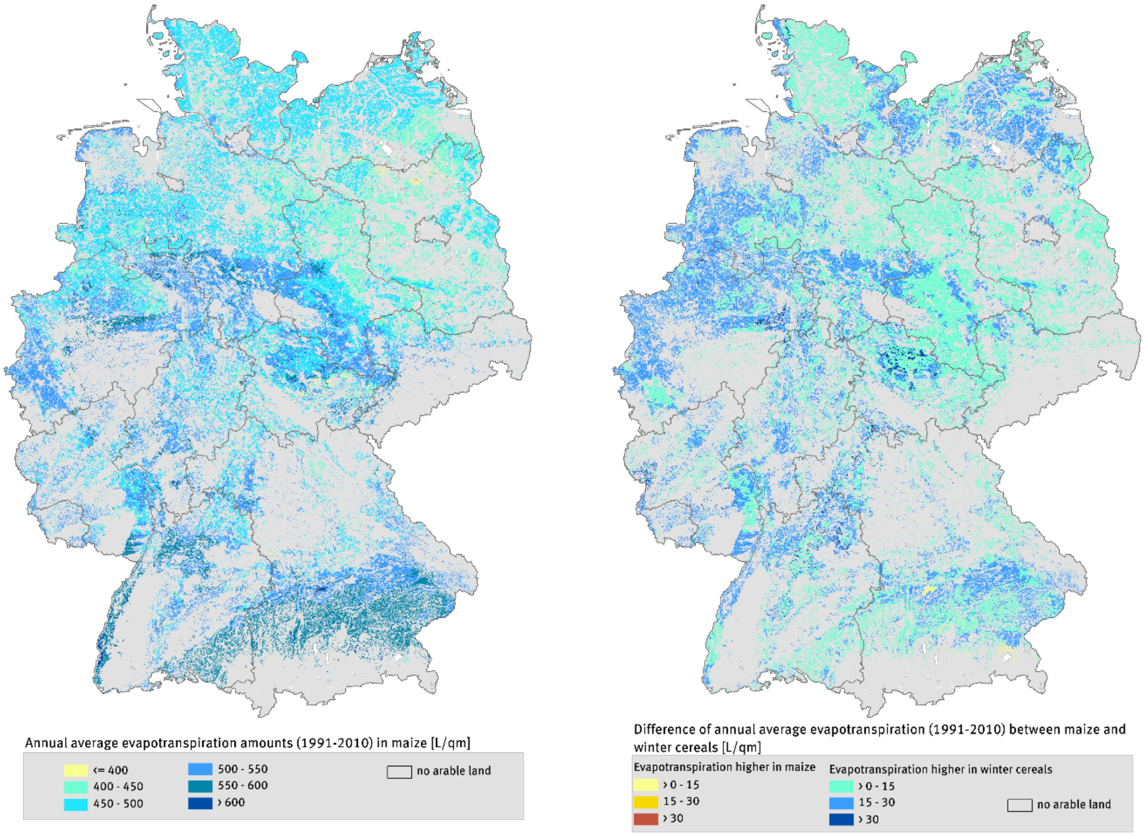
Results of the simulated soil water regime are analysed considering the stepwise modelling approach presented in the previous section. The evaluation covers all parts of the soil water balance. For the analysis, results of GeoPELMO DE are presented considering the internal post-processing modules. Where appropriate, the focus is placed on the effect of switching on/off individual processes like runoff, macropore flow and drainage to illustrate the impact of specific processes on the nationwide spatially distributed modelling results of the soil water regime. In the following chapter, the influence of runoff and drainage on the soil water balance is discussed in more detail. Furthermore, specific evaluations are provided according to the simulated percolate amounts depending on different soil water processes and crops.

5.3.1 Evapotranspiration

GeoPELMO DE calculates the actual evapotranspiration based on the daily potential evapotranspiration and the soil moisture content in the root zone Figure 52 shows the spatial distribution of actual evapotranspiration for the two different crops maize and winter cereals when the FOCUS modelling routine of chromatographic flow is used and all additional processes are switched off [FOCUS L]. Because the crop growth influences the amount of water in soil, different spatial results are calculated dependent on the crop. However, for winter cereals and maize the effect on the actual evapotranspiration is not very pronounced. The background is that during the time with the biggest difference between these crops (winter dormancy period for winter cereals, bare soil for maize), the actual evapotranspiration is close to zero because of low temperatures. The main driving factor for actual evapotranspiration is rainfall. While the precipitation maps show a clear west-east gradient (see Figure 8 in chapter 4.2.2), the distribution of actual evapotranspiration shows in addition a north-south gradient, which is presumably due to differences in soil types. The calculated differences in evapotranspiration between the two crops are in the classes 0-15 L/m^2 and 15-30 L/m^2 for most agricultural soils. In some minor areas, differences above 30 L/m^2 are estimated.

It is demonstrated in Table 43 for maize and in Table 44 for winter cereals that only runoff has a minor effect on the spatially distributed amount of modelled annual evapotranspiration. However, the effect is rather small (about 1 % to 2 % reduction). Evapotranspiration is calculated in PELMO based on a triangular function that gives the maximum weight to the soil moisture close to the soil surface. Runoff is a process which changes the soil moisture content at the soil surface. Consequently, runoff slightly reduces evapotranspiration while the other processes like preferential flow and drainage don’t change it because their influence on the soil moisture content is either too small (e.g. macropore flow) or only important at deeper soil layers (drainpipe flow).

Figure 52: **Annual average evapotranspiration calculated with GeoPELMO DE depending on different crop covers**



Source: own illustration, Fraunhofer IME

Table 43: **Influence of runoff, macropore flow and drainage on the spatially distributed annual actual evapotranspiration modelled with GeoPELMO DE in maize**

Evapotranspiration [L/m^2]	FOCUS L	FOCUS L+R	FOCUS L+R+M	FOCUS L+R+M+D	FOCUS L+R+M+D*
Median	489.3	482.5	482.9	482.9	482.9
80th percentile	532.9	527.0	527.7	527.6	527.6
90th percentile	558.9	554.2	555.1	555.1	555.1
95th percentile	574.1	570.0	569.8	569.8	569.8
99th percentile	595.8	594.3	594.1	594.1	594.1
100th percentile	701.8	690.2	688.9	688.9	688.9

The abbreviations for the various simulation runs correspond to the explanations in chapter 5.1.2. In the last simulation run*, an organic carbon content of 0.2 % was used for all soil horizons of class h0 independent of their soil depth.

Table 44: **Influence of runoff, macropore flow and drainage on the spatially distributed annual actual evapotranspiration modelled with GeoPELMO DE in winter cereals**

Evapotranspiration [L/m²]	FOCUS L	FOCUS L+R	FOCUS L+R+M	FOCUS L+R+M+D	FOCUS L+R+M+D*
Median	504.1	499.7	500.0	499.9	499.9
80th percentile	549.4	547.8	547.6	547.6	547.6
90th percentile	573.6	571.6	571.6	571.6	571.6
95th percentile	587.1	585.5	585.6	585.6	585.6
99th percentile	610.1	608.8	608.9	608.9	608.9
100th percentile	719.5	714.8	714.2	714.2	714.2

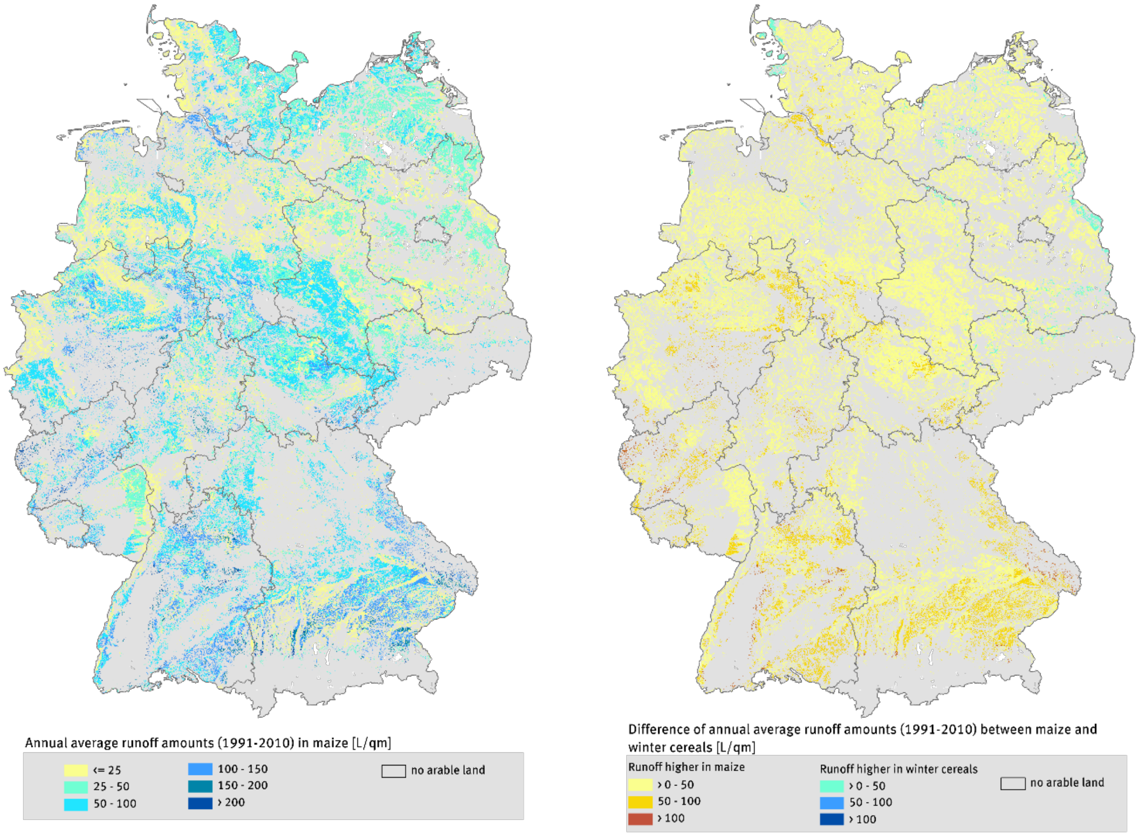
The abbreviations for the various simulation runs correspond to the explanations in chapter 5.1.2. In the last simulation run*, an organic carbon content of 0.2 % was used for all soil horizons of class h0 independent of their soil depth.

5.3.2 Runoff

GeoPELMO DE calculates the runoff based on the runoff curve number approach (see chapter 4.4). Runoff events are simulated on a daily time step. Figure 53 shows the spatial distribution of runoff amounts for two different crops maize and winter cereals when the FOCUS modelling routine of chromatographic flow is used and other processes like macropore flow and drainage are switched off [FOCUS L+R]. Because runoff curve numbers are dependent on the crop growth, two different crops are calculated for comparison. Higher amounts of runoff are simulated in maize than in winter cereals due to fallow conditions during the autumn and winter periods. The respective ranges of runoff in these crops are 5 L/m² to 50 L/m² and 5 L/m² to 100 L/m² for winter cereals and maize, respectively. The calculated differences of annual runoff quantities between the two crops are in the class 0-50 L/m²for most agricultural soils. In some areas in central and southern Germany, differences of up to 100 L/m² and even more are estimated.

In Table 45 the influence of macropore flow on averaged annual runoff is presented for maize and winter cereals. The analysis is based on a comparison of results from two simulation runs FOCUS L+R and FOCUS L+R+M from the sequential modelling approach. About a maximum of 10 % reduction of runoff is calculated when macropore flow is considered in the simulation. The effect is relatively small, and different crops do not have a substantial influence on the reduction of runoff. The modelling effect of drainage on runoff is not discussed since drainage only affects the soil water at deeper soil layers and not at the soil surface. It is therefore not likely that drainpipe flow would change surface runoff results in GeoPELMO DE.

Figure 53: Annual runoff amounts calculated with GeoPELMO DE depending on different crop covers



Source: own illustration, Fraunhofer IME.

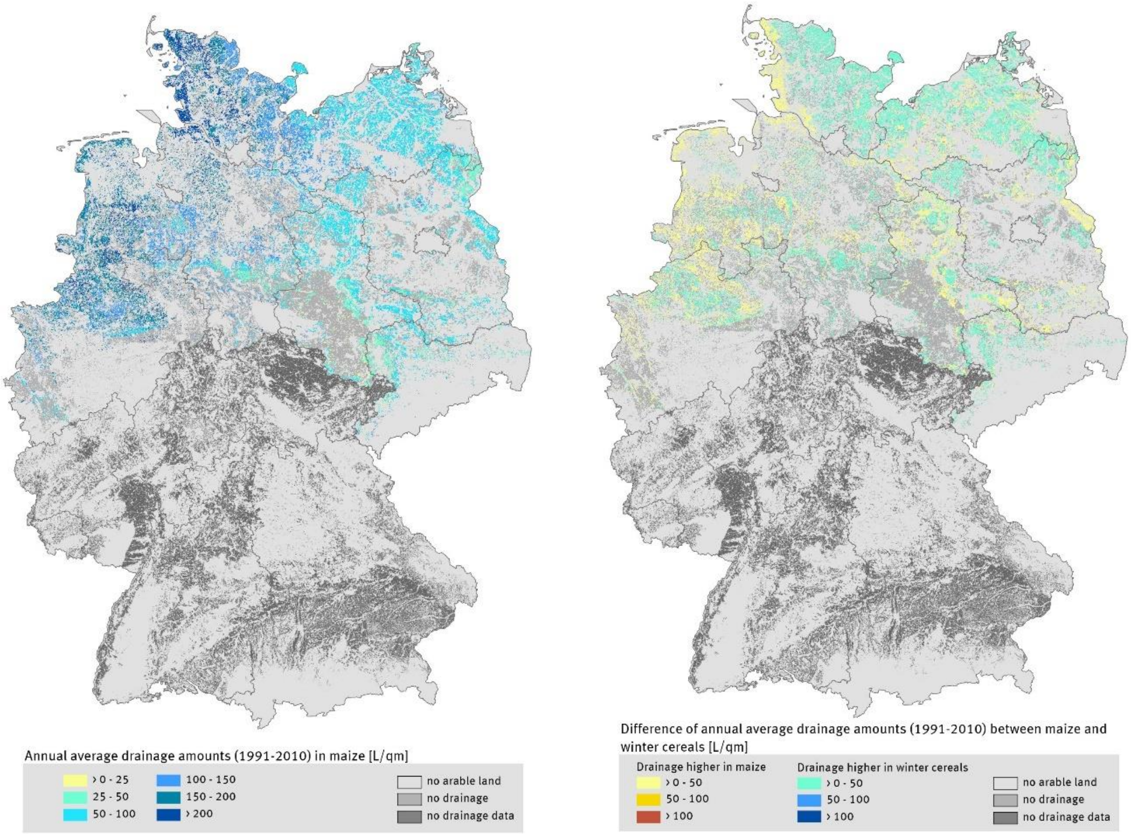
Table 45: Influence of macropore flow on spatial distributed average annual runoff amounts modelled with GeoPELMO DE in maize and winter cereals

Runoff	Maize FOCUS L+R [L/m²]	Maize FOCUS L+R+M [L/m²]	Maize Reduction [%]	Winter cereals FOCUS L+R [L/m²]	Winter cereals FOCUS L+R+M [L/m²]	Winter cereals Reduction [%]
Median	41.7	37.4	10.4	19.3	17.4	10.0
80th percentile	79.2	74.2	6.4	37.1	33.8	9.0
90th percentile	102.3	93.9	8.2	47.7	44.3	7.1
95th percentile	124.1	112.3	9.6	59.5	51.9	12.8
99th percentile	166.3	159.1	4.3	83.4	81.1	2.7
100th percentile	406.5	406.4	0	188.4	188.3	0

5.3.3 Drainage

The parametrisation of drainage in GeoPELMO DE is presented in chapter 4.5.5. The maps presented in Figure 54 show the spatial distribution of annual water in drainage system when maize and winter cereals are cropped. The dark grey colours in the maps represent the areas in southern Germany where drainage has not been considered in GeoPELMO DE, because data were not available. The light grey colours represent the areas where drainage has not been considered in GeoPELMO DE because the areas are potentially not drained. Hardly any differences can be found when the average annual water in drainage systems is compared for both crops. This is confirmed by statistical information about the spatial distribution of estimated annual water amounts in drainage systems in Table 46. The 80th percentile was simulated to be 142.8 L/m^2 and 144.4 L/m^2 in maize and winter cereals, respectively. The median was 0 since in more than 50 % of the agricultural land no drainage systems are considered in GeoPELMO DE. The maximum estimated annual drain water flow was about 370 L/m^2. However, the results further demonstrate that the simulated drainage water flow is very much dependent on the season. The differences in spring and summer month (March to August) compared to autumn and winter months (September to February) are shown in Figure 55 and Figure 56 for maize and winter cereals, respectively. The figures demonstrate that higher drainage rates are always modelled during autumn and winter month. Furthermore, a decreasing gradient of these seasonal differences in drainage rates from west to east is visible in Northern Germany for both investigated crops.

Figure 54: Annual drainage amounts calculated with GeoPELMO DE depending on different crop covers

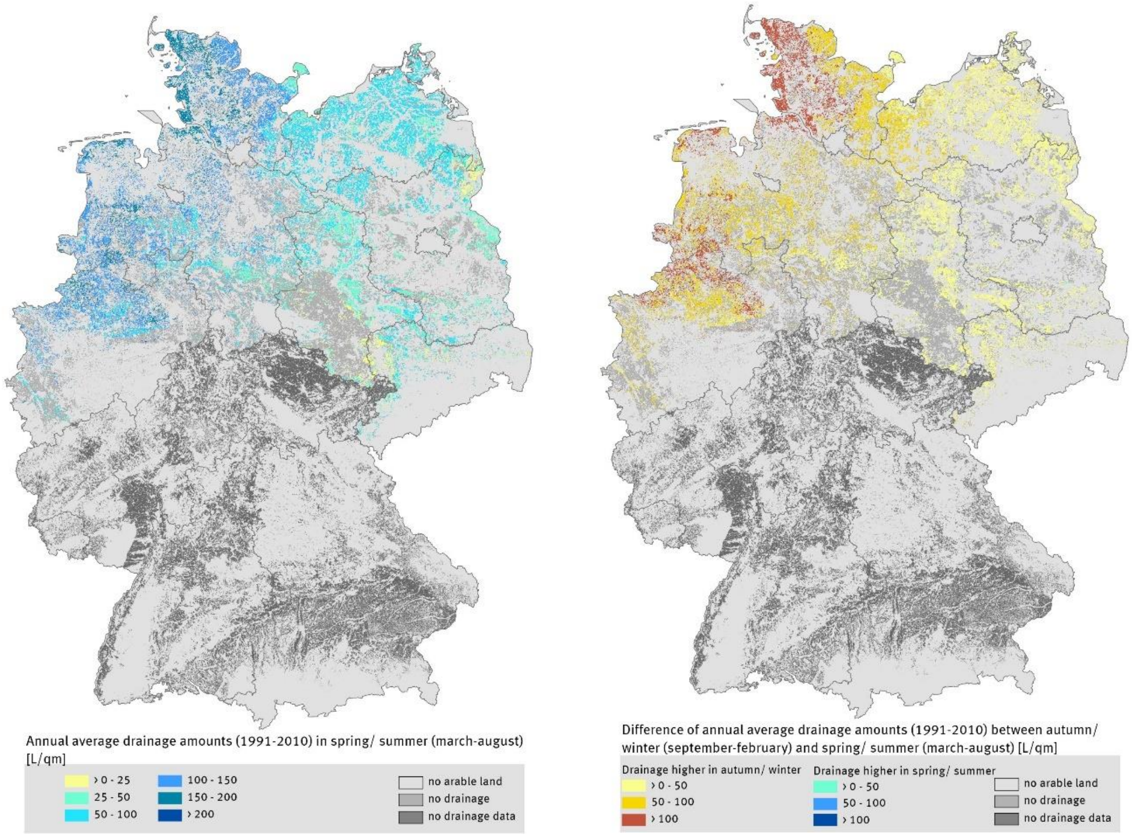


Source: own illustration, Fraunhofer IME.

Table 46: Statistical analysis of the spatial distribution of annual water in drainage systems

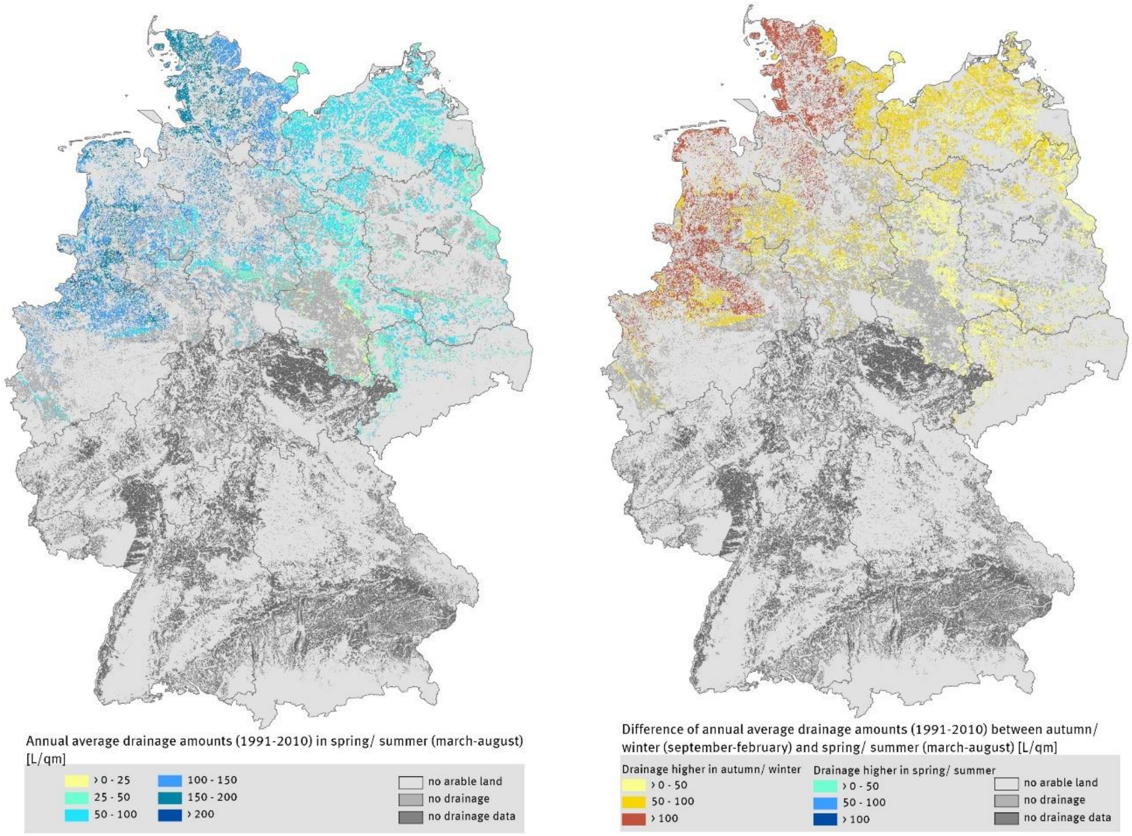
Runoff	Maize FOCUS L+R+M+D [L/m²]	Winter cereals FOCUS L+R+M+D [L/m²]
Median	0	0
80th percentile	80.5	82.6
90th percentile	142.8	144.4
95th percentile	184.4	182.9
99th percentile	219.4	217.0
100th percentile	367.4	369.2

Figure 55: Seasonal drainage amounts in spring/summer and autumn/winter calculated with GeoPELMO DE for maize



Source: own illustration, Fraunhofer IME.

Figure 56: Seasonal drainage amounts in spring/summer and autumn/winter calculated with GeoPELMO DE for winter cereals



Source: own illustration, Fraunhofer IME.

Table 47 provides different percentiles of the spatial distribution of the estimated drainage flow in spring, summer and autumn, winter for both crops. The results provide evidence that drainage flow in the autumn and winter periods is much more important with about three times higher drain flow amounts than in the spring and summer period. Furthermore, the percentile analysis confirms that differences of drainage between both modelled crops are only minor compared to seasonal influences.

Table 47: Percentile analysis of the spatially distributed seasonal drainage flow

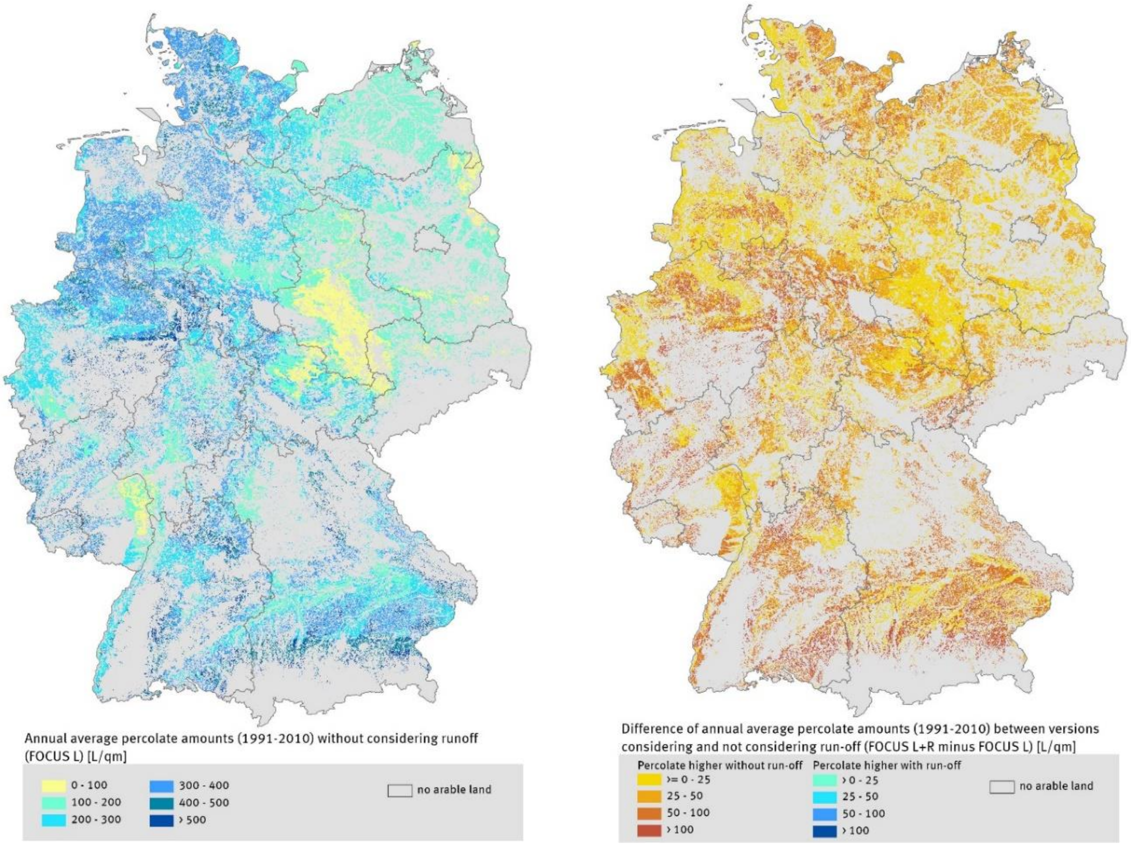
Runoff	Maize FOCUS L+R+M+D Sept.-Feb. [L/m²]	Maize FOCUS L+R+M+D March - Aug [L/m²]	Winter cereals FOCUS L+R+M+D Sept. – Feb. [L/m²]	Winter cereals FOCUS L+R+M+D March – Aug [L/m²]
Median	0	0	0	0
80th percentile	62.0	19.1	67.6	15.6
90th percentile	108.8	31.7	117.5	26.7
95th percentile	141.8	41.3	149.8	35.6
99th percentile	170.1	53.4	173.7	45.8
100th percentile	270.7	96.7	277.6	112.4

5.3.4 Percolate

In the following, nationwide estimated percolate amounts in the unsaturated soil zone from different simulation runs of the stepwise modelling approach with GeoPELMO DE are compared with each other and with published values from the German Hydrological Atlas (map 4.5 in HAD 2003, Jankiewicz et al. 2005). The analysis is intended to show the influence of runoff and drainage on the percolate water volume distribution and the plausibility of the new spatial distributed model version of PELMO in general. The comparison is always carried out based on calculations for the two crops maize and winter cereals.

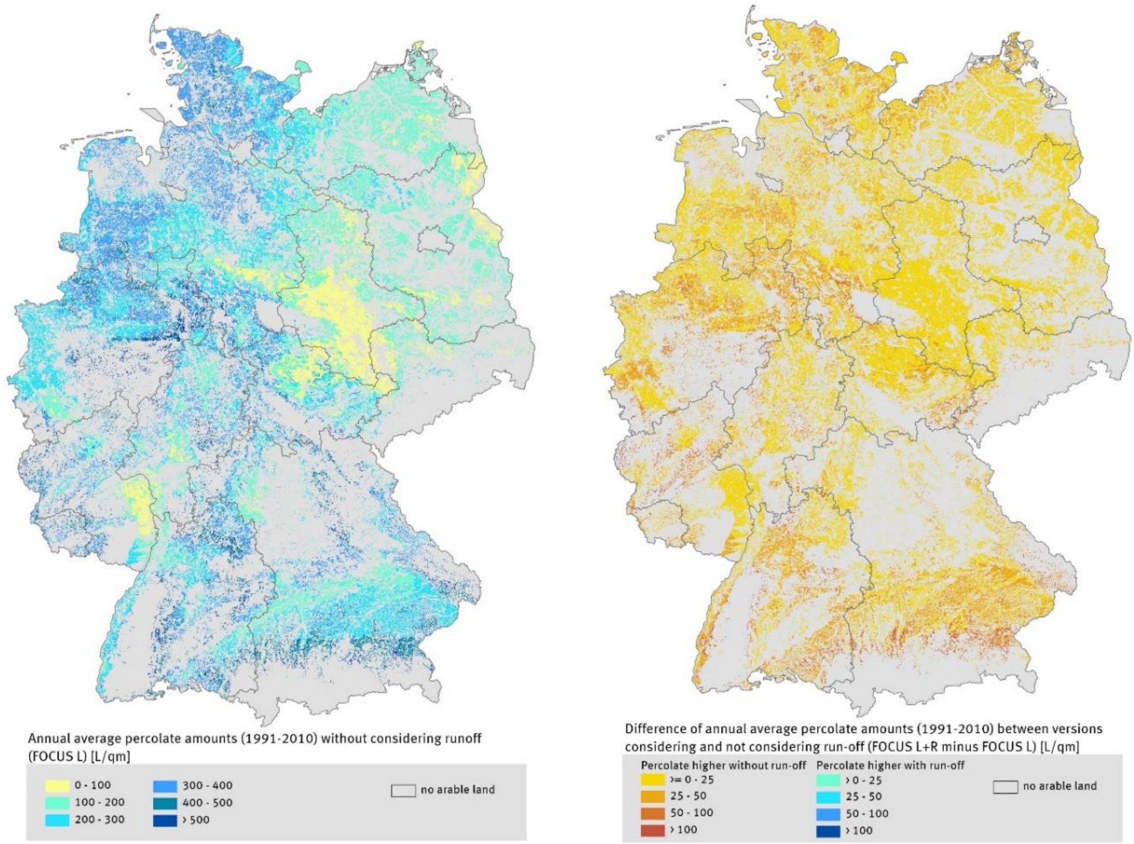
The influence of runoff on the spatial distributions of averaged annual the percolate volumes in Germany when maize and winter cereals are cultivated are presented in Figure 57 and Figure 58, respectively. In both figures, the nationwide distribution of annual percolate volumes is provided as map when runoff is not considered (maps on the left). In addition, the nationwide distribution of the difference in percolate volumes was calculated dependent on whether runoff was considered or not (maps on the right). As expected, lower percolate volumes are simulated when runoff is considered in the simulations. However, the impact of runoff on the annual percolate amounts is rather limited and there are only minor differences between both crops. That means that runoff amounts are in the same range as the reduction of percolate volumes due to runoff. That supports the previous conclusion that even evapotranspiration doesn't dependent very much on whether runoff is considered in the simulation or not (see Table 43 and Table 44).

Figure 57: Influence of runoff on percolate amounts at 1 m soil depth calculated with GeoPELMO DE for maize



Source: own illustration, Fraunhofer IME.

Figure 58: Influence of runoff on percolate amounts at 1 m soil depth calculated with GeoPELMO DE for winter cereals



Source: own illustration, Fraunhofer IME.

In the next step, the contribution of macropore flow to the averages annual percolate volumes was evaluated when maize and winter cereals are cultivated. Finally, the influence of macropore flow on the total amount of percolate is negligible in both crops as shown in Table 48.

Table 48: Influence of macropore flow on annual percolate amounts at 1 m soil depth calculated with GeoPELMO DE in maize and winter cereals

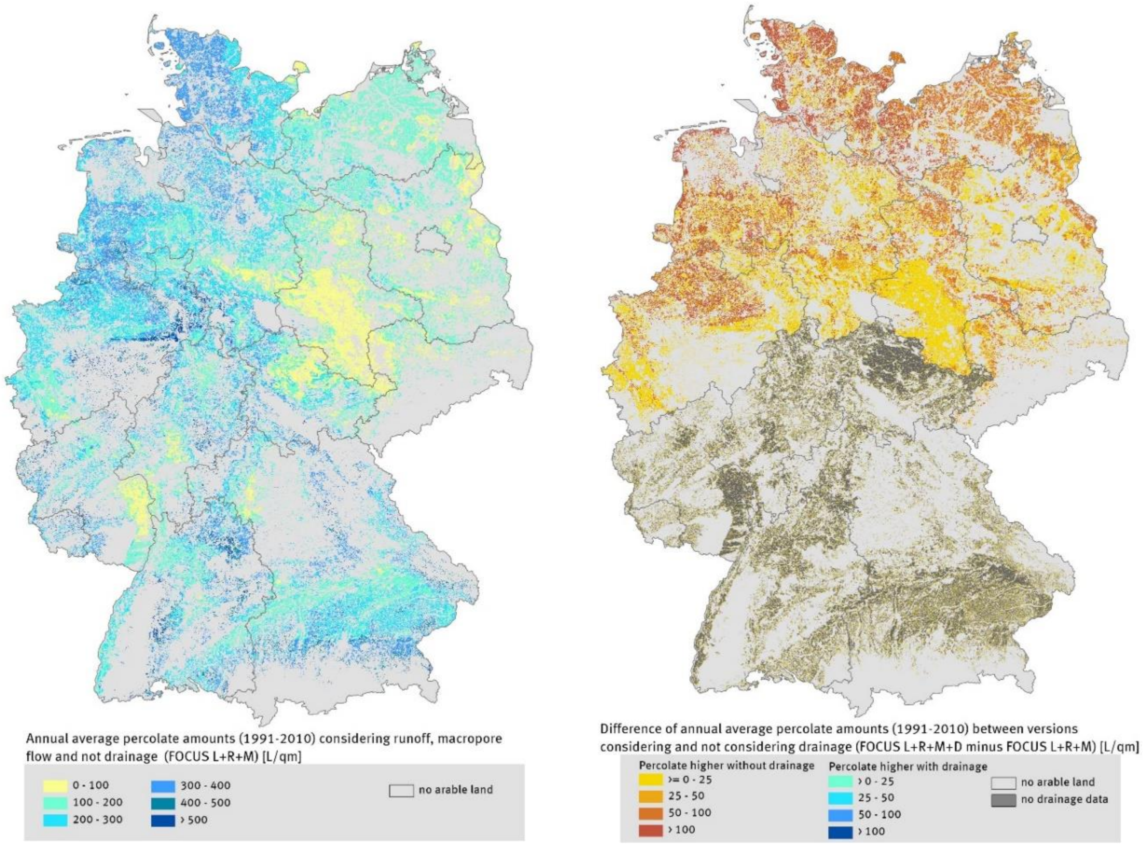
Percolate	Maize FOCUS L+R [L/m^2]	Maize FOCUS L+R+M* [L/m^2]	Maize difference [%]	Winter cereals FOCUS L+R* [L/m^2]	Winter cereals FOCUS L+R+M* [L/m^2]	Winter cereals difference [%]
Median	201.6	202.5	0.5	207.2	210.6	1.6
80th percentile	303.3	305.8	0.8	311.7	315.4	1.2
90th percentile	350.5	355.0	1.3	366.8	370.5	1.0
95th percentile	398.6	395.2	-0.9	418.1	415.8	-0.5
99th percentile	530.8	530.9	0.0	596.4	595.1	-0.2
100th percentile	909.5	909.7	0.0	1009.1	1009.2	0.0

* Simulations with minimum 4% and maximum 8% fraction for macro-pores in high macro-pore regions

If preferential flow is considered by modelling, a difference of around 1 % of the annual percolate volume is calculated. As the effect is very small, the spatial distribution of percolate as a function of macropore flow is not further shown in maps. There was also no difference of the annual percolate volume when the macropore parametrisation was changed (i.e., minimum and maximum fraction of macropores). However, the different parametrisation influenced the concentrations in the percolate (see next section).

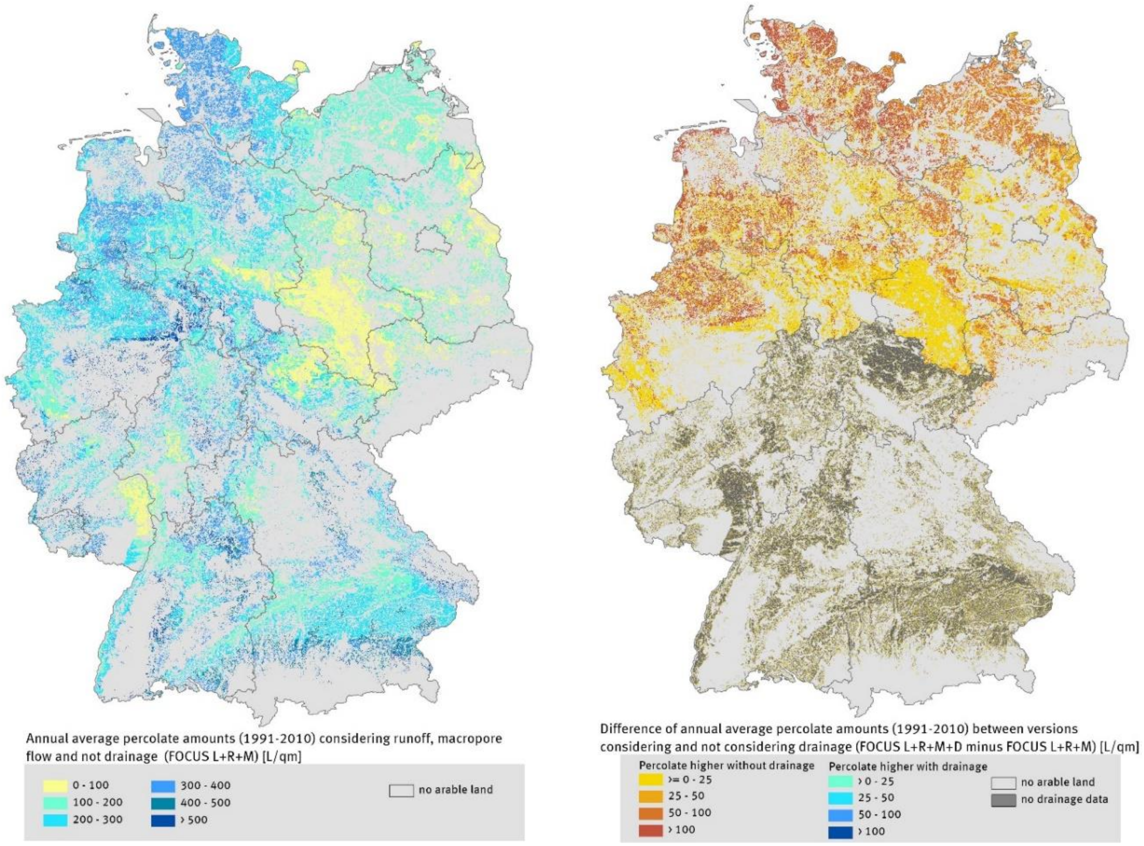
In comparison, drainage has a greater influence on the annual percolate water volume. This is demonstrated in Figure 59 and Figure 60 when maize and winter cereals are cultivated, respectively. In both figures, the nationwide distribution of annual percolate volumes is provided as map when runoff, macropore flow and potential artificial drainage are considered in Northern Germany (map on the left). In addition, the nationwide distribution of the difference in percolate volumes was calculated dependent on whether drainage was considered or not (map on the right). The light grey colours in the maps represent the areas in southern Germany where drainage systems have not been considered in GeoPELMO DE. As expected, lower percolate volumes are simulated when drainage is considered in the simulations.

Figure 59: Influence of drainage on percolate amounts at 1 m soil depth calculated with GeoPELMO DE for maize



Source: own illustration, Fraunhofer IME.

Figure 60: **Influence of drainage on percolate amounts at 1 m soil depth calculated with GeoPELMO DE for winter cereals**



Source: own illustration, Fraunhofer IME.

In addition, some percentile analysis of the nationwide spatial distribution of annual percolate volumes are presented to compare for both maize and winter cereals in Table 49 when all additional processes are included in the modelling routine. The absolute differences between both crops are minor but they increase with increasing percolate amounts (median: 5.8 L/m², 100th percentile: 99.6 L/m²).

Table 49: **Statistical analysis of the spatial distribution of annual percolate volumes for maize and winter cereals considering runoff, macropore flow and drainage**

Percolate	Maize FOCUS L+R+M+D [L/m²]	Winter cereals FOCUS L+R+M+D [L/m²]	Difference [%]
Median	147.5	153.3	5.8
80th percentile	281.1	290.6	9.4
90th percentile	341.5	353.6	12.1
95th percentile	389.5	414.1	24.5
99th percentile	529.2	594.5	65.3
100th percentile	909.7	1009.2	99.5

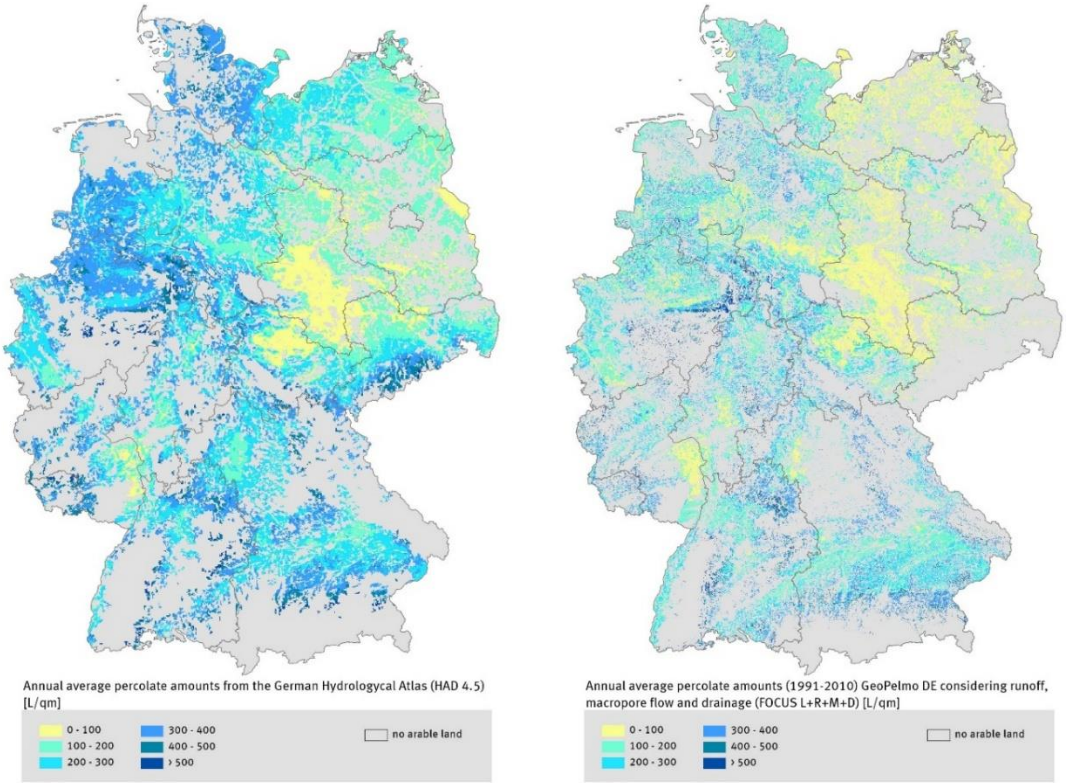
Table 46 already showed the spatial distribution of the annual drainage flow in percentiles, which for both calculated crops is zero in the median and increases in the higher percentiles up to a maximum of 370 L/m^2. These values are listed again in Table 50. In addition, the absolute and relative difference in the distribution of percolate volumes as a function of drainage flow is shown in percentiles. The results show that although the spatial median of the annual percolate is 0 (meaning that less than 50 % of the agricultural area have potential drainage systems), the relative difference of the median of the percolate amounts with and without drainage is about 27 %. The background for this discrepancy is the different locations which are considered when calculating the medians with and without drainage. Both sites are characterised by different climatic conditions. Furthermore, the absolute and relative differences between the percolate volumes decrease with increasing percentile when modelling runs with and without considering drainage are compared. This is because the fields with the highest percolate volumes do not contain any potential artificial drainage systems. This is shown, for example, by the fact that regardless of whether drainage systems were included in the GeoPELMO DE simulation or not, the maximum percolate in the map (i.e., Freudenstadt) is characterised by 910 L/m^2 and 1009 L/m^2 when maize or winter cereals are grown, respectively. The field with a maximum drainage flow of 368 L/m^2 is represented by a completely different location (i.e., Lüdenscheid).

Table 50: Influence of drainage on the spatially distributed annual percolate volumes modelled with GeoPELMO DE in maize and winter cereals

Percolate	Maize difference of percolate due to drainage [%]	Maize difference of percolate due to drainage [L/m²]	Maize drainage [L/m²]	Winter cereals difference of percolate due to drainage [%]	Winter cereals difference of percolate due to drainage [L/m²]	Winter cereals drainage [L/m²]
Median	-27.2	-55.0	0	-27.2	-57.3	0
80th percentile	-8.1	-24.7	80.5	-7.9	-24.8	82.6
90th percentile	-3.8	-13.5	142.8	-4.6	-16.9	144.4
95th percentile	-1.4	-5.7	184.4	-0.4	-1.8	182.9
99th percentile	-0.3	-1.7	219.4	-0.1	-0.7	217.0
100th percentile	0	0	367.4	0	0	369.2

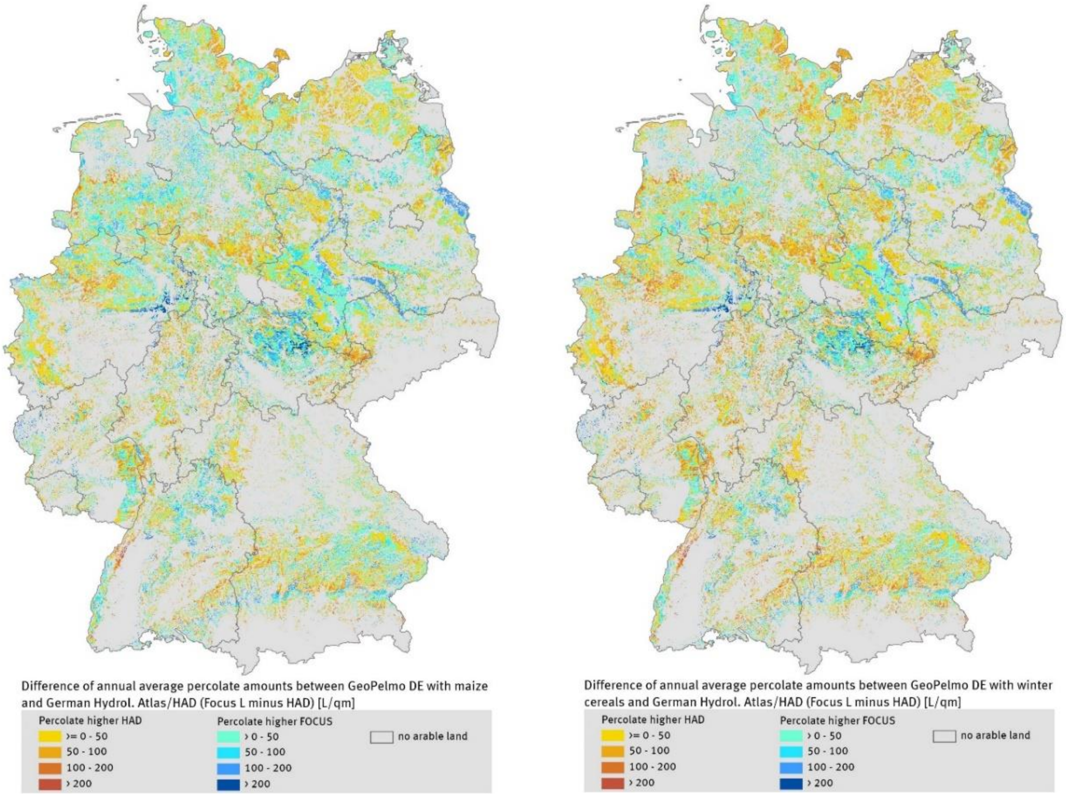
In the following, percolate amounts of different modelling approaches are compared. The maps in Figure 61 show a similar nationwide distribution of percolate amounts modelled with GeoPELMO DE (FOCUS L parametrisation without runoff, preferential flow and drainage according to step 1 in section 5.2) in comparison to the calculations in the German Hydrological Atlas (map 4.5 in HAD 2003), especially in the North-South and West-East gradients. Regional deviations are caused by the fact that both approaches consider different geodata and modelling algorithms.

Figure 61: Comparison of percolate amounts in the unsaturated soil zone from different modelling approaches



Source: own illustration, Fraunhofer IME.

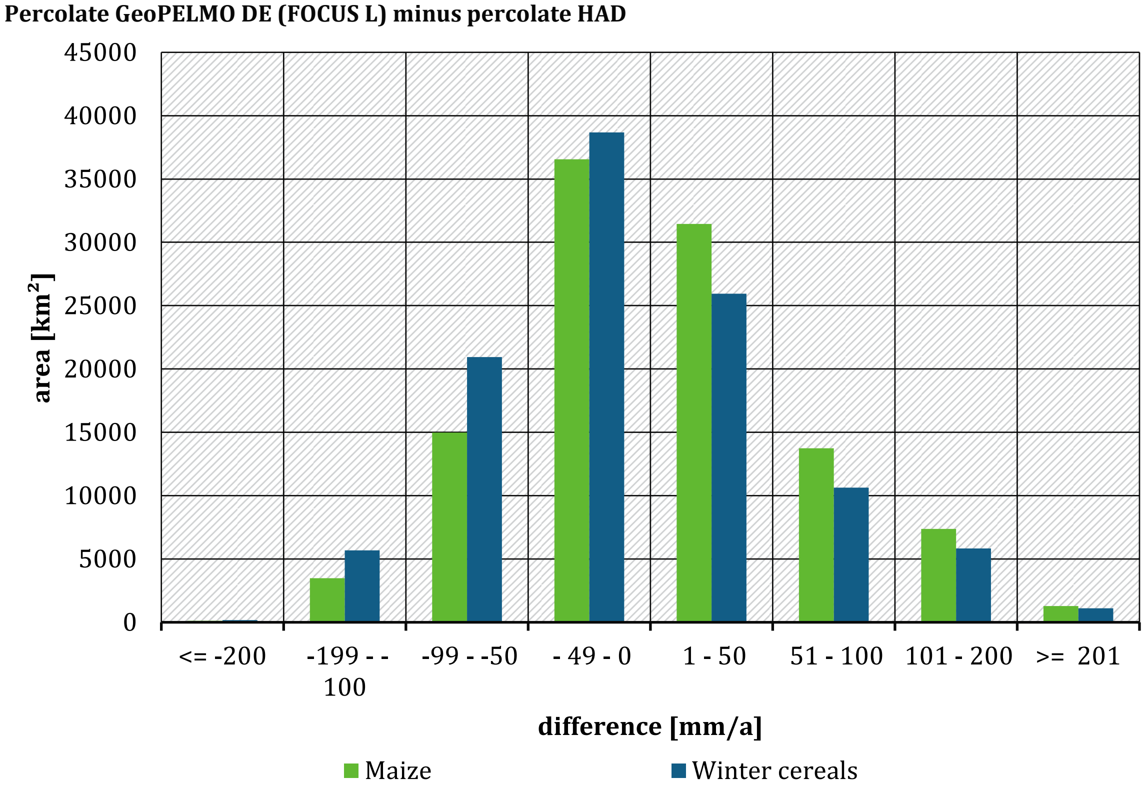
Figure 62: Percolate amounts in the unsaturated soil zone calculated with GeoPELMO DE compared to the German Hydrological Atlas (map 4.5)



Source: own illustration, Fraunhofer IME.

In Figure 63 the calculated difference between the percolate amount modelled with GeoPELMO DE under maize and winter cereals cropping and the percolate amount published in map 4.5 of the HAD (2003) is shown. The main part of the agricultural area shows differences up to +/- 50 mm/a. Minor parts are represented by differences of percolate volumes between 50 and 100 mm/a and 100 and 200 mm/a in both directions. For only very view agricultural areas differences of average annual percolate amounts above 200 mm are estimated (see also diagram in Figure 63). This confirms that the percolate amounts modelled with GeoPELMO DE (FOCUS L: chromatographic flow without considering runoff, preferential flow and drainage) are quite comparable to the soil percolate amounts provided in the HAD (2003) and spatial deviations are almost equally distributed.

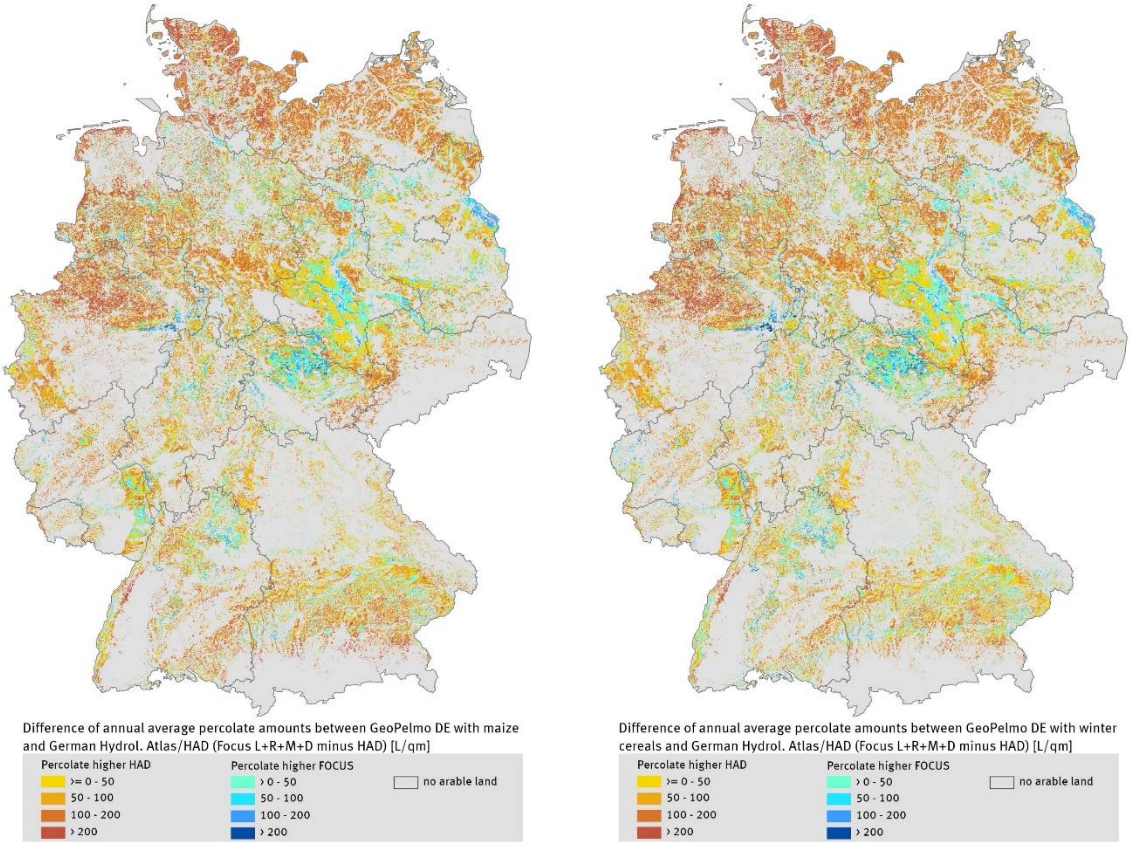
Figure 63: Deviations of average annual percolate amounts between GeoPELMO DE (FOCUS L in maize and winter cereals) and the German Hydrological Atlas (map 4.5)



Source: own illustration, Fraunhofer IME.

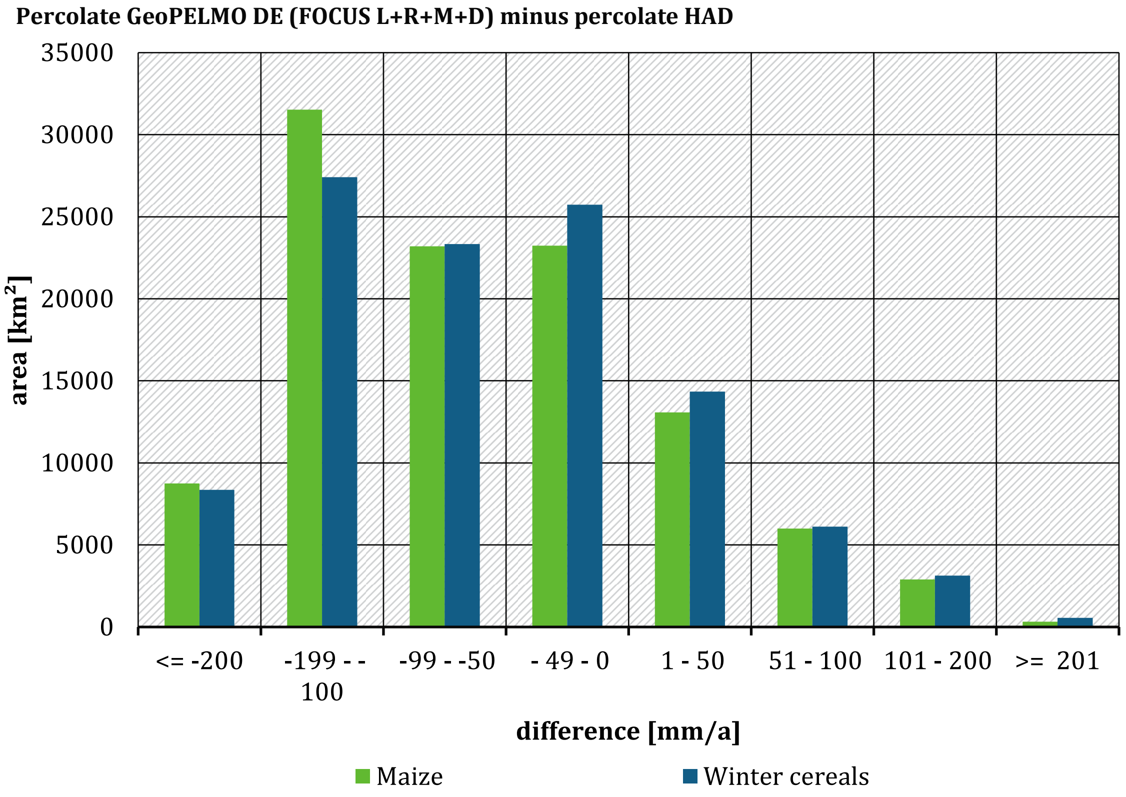
The same spatial analysis is provided for nationwide percolate amounts simulated with GeoPELMO DE when additional processes like runoff, macropore flow and drainage flow are considered (FOCUS L+R+M+D parametrisation according to step 4 in section 5.2). The results are provided for maize and winter cereals in Figure 64 and Figure 65. It can be observed that for both crops lower average annual percolate volumes are estimated with GeoPELMO DE (FOCUS L+R+M+D) compared to the German Hydrological Atlas for most of the agricultural area. Only minor regions, mainly located in the eastern part of Germany are represented with higher percolate amounts when PELMO is used and all additional processes are considered. The differences in the leachate quantities between GeoPELMO DE and the map 4.5 of the HAD are no longer almost equally distributed but show a left-skewed systematic deviation. This underlines the conclusion made before that the nationwide percolate amounts calculated by GeoPELMO DE are noticeable reduced when additional processes like runoff and drainage are considered.

Figure 64: Percolate amounts in the unsaturated soil zone calculated with GeoPELMO DE compared to the German Hydrological Atlas (map 4.5)



Source: own illustration, Fraunhofer IME.

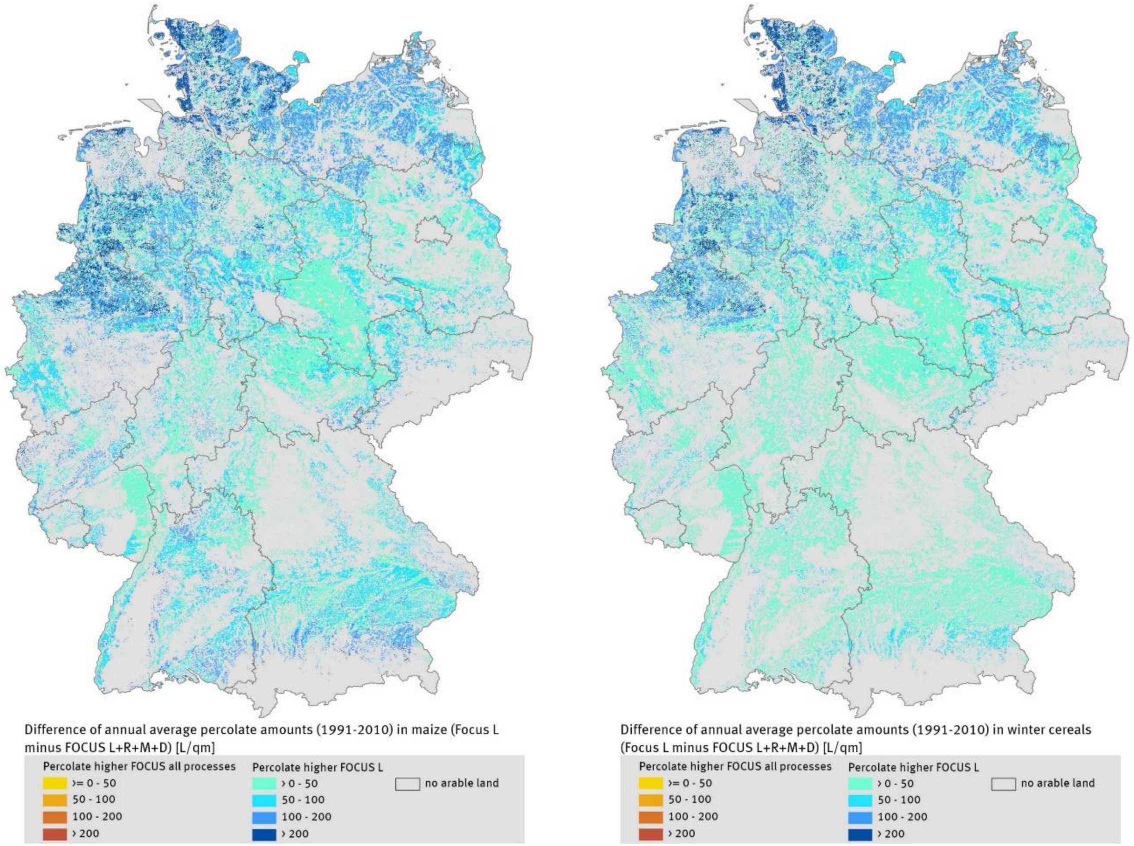
Figure 65: **Deviations of average annual percolate amounts between GeoPELMO DE (FOCUS L+R+M+D in maize and winter cereals) and the German Hydrological Atlas (map 4.5)**



Source: own illustration, Fraunhofer IME.

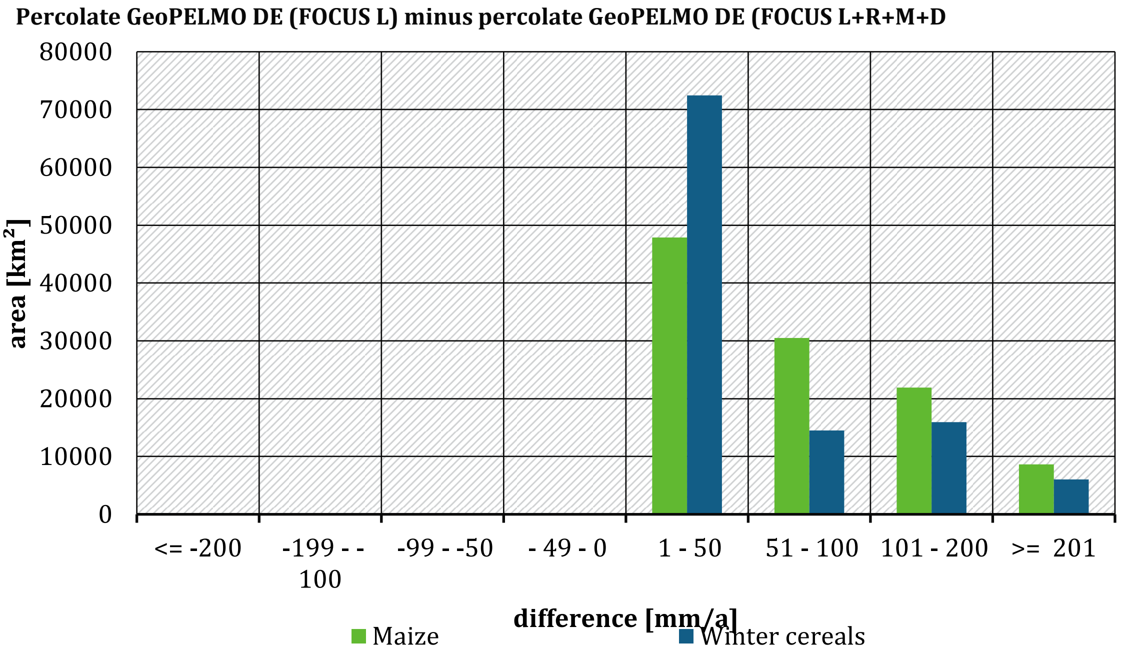
To quantify the differences of percolate amount between GeoPELMO DE calculations based on the FOCUS approach (FOCUS L) and with including additional water balance processes like runoff, macropore and drainage flow (FOCUS L+R+M+D) both result datasets were subtracted. Figure 66 and Figure 67 shows the spatial deviations of nationwide percolate volumes from both GeoPELMO DE model versions for maize and winter cereals. The analysis provides evidence that the percolate amounts are always lower when the three additional water balance processes are considered. For most of the agricultural area a difference of percolate volumes between 0 and 50 mm/a is estimated for both crops, maize and winter cereals, mainly in central and southern Germany. In the northern and north-western part of Germany estimated differences can be even higher up to 200 mm/a and more. This is linked to the implementation of drainage in PELMO, where potentially drained areas have been identified primarily for unconsolidated rock areas in Northern Germany.

Figure 66: Comparison of percolate amounts in the unsaturated soil zone calculated with different model versions of GeoPELMO DE



Source: own illustration, Fraunhofer IME.

Figure 67: Deviations of average annual percolate amounts between GeoPELMO DE (FOCUS L) and GeoPELMO DE (FOCUS L+R+M+D) in maize and winter cereals



Source: own illustration, Fraunhofer IME.

To summarise, the version of GeoPELMO DE based on the FOCUS model approach (FOCUS L) calculates soil percolate leachate volumes of the same order of magnitude as provided in the German Hydrological Atlas (map 4.5 in HAD 2003). Spatial deviations are equally distributed on nationwide level between the two different approaches and are mainly in the order of up to +/- 50 mm/a, but can also be higher in individual regions. The implementation of the processes runoff, macropore flow and drainage flow in PELMO significantly reduces the calculated percolate quantities in total, whereby the influence of the macropore flow is rather small and negligible. The deviations from the leaching amounts in the HAD (2003) are larger and more systematic due to the implementation of runoff and drainage.

5.4 Results for percolate concentrations

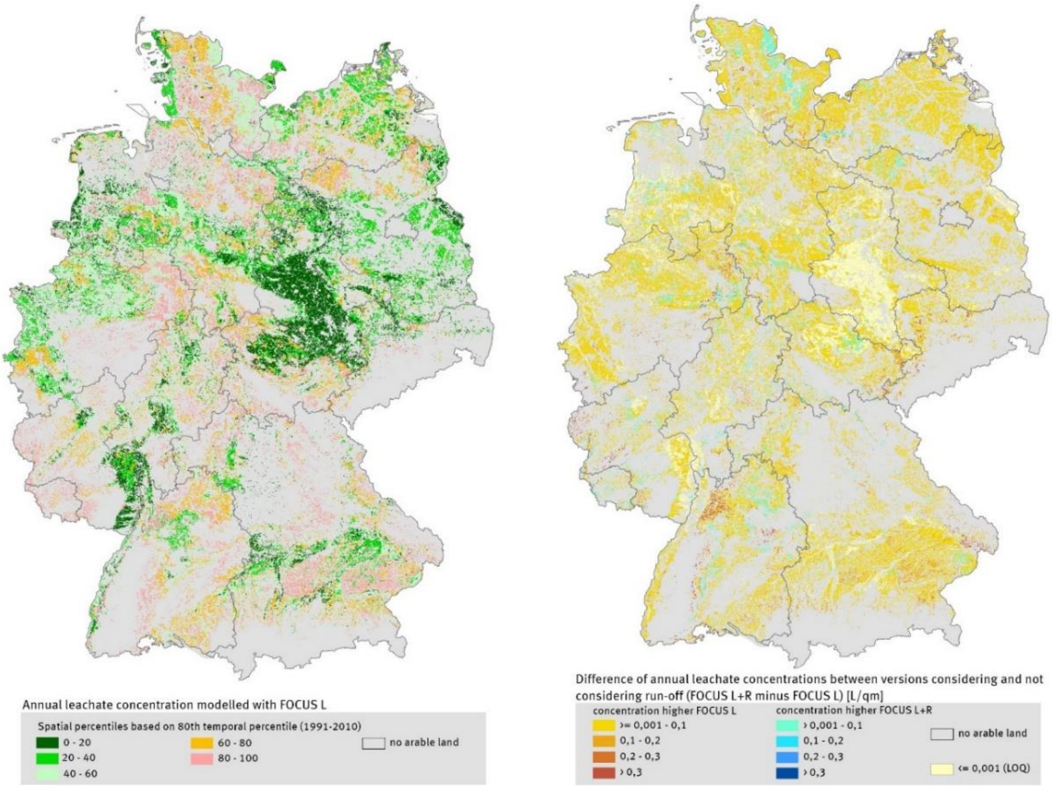
The simulated spatially distributed percolate concentrations for dummy active substances and metabolites are analysed in the following considering the stepwise modelling approach presented in section 5.2. The evaluation is intended to provide evidence on the effect of new model parametrisations in GeoPELMO DE for estimating leachate concentrations in 1 m depth of the unsaturated soil zone by adding runoff, macropore flow and drainage into the FOCUS modelling routine and by replacing the humus soil class H0 with different default values for organic carbon contents in agricultural subsoils. All evaluations are provided for the two crops maize and winter cereals to cover different seasonal effects.

5.4.1 Active substances

Nationwide average annual percolate concentrations are calculated and evaluated for the three different fictive parent compounds (P1, P2, P3), whose properties differ in their sorption constants and their degradation rate in soil (see section 5.1). Maps are provided as example for the dummy active substance P2, which is moderately mobile and fast degrading. In the maps on the left, the spatially distributed annual leachate concentrations are shown as relative figures in five percentile classes based on the 80th temporal percentile according to 20 weather years. The maps on the right show the difference in leachate concentrations depending on the different parameterisation of the model. The aim is to visualise the spatial effect of the additional processes like runoff, macropore flow and artificial drainage flow in Germany. The tables in this chapter contain statistical values such as the median and 80th percentile of the spatially varying concentrations for all three calculated dummy active substances.

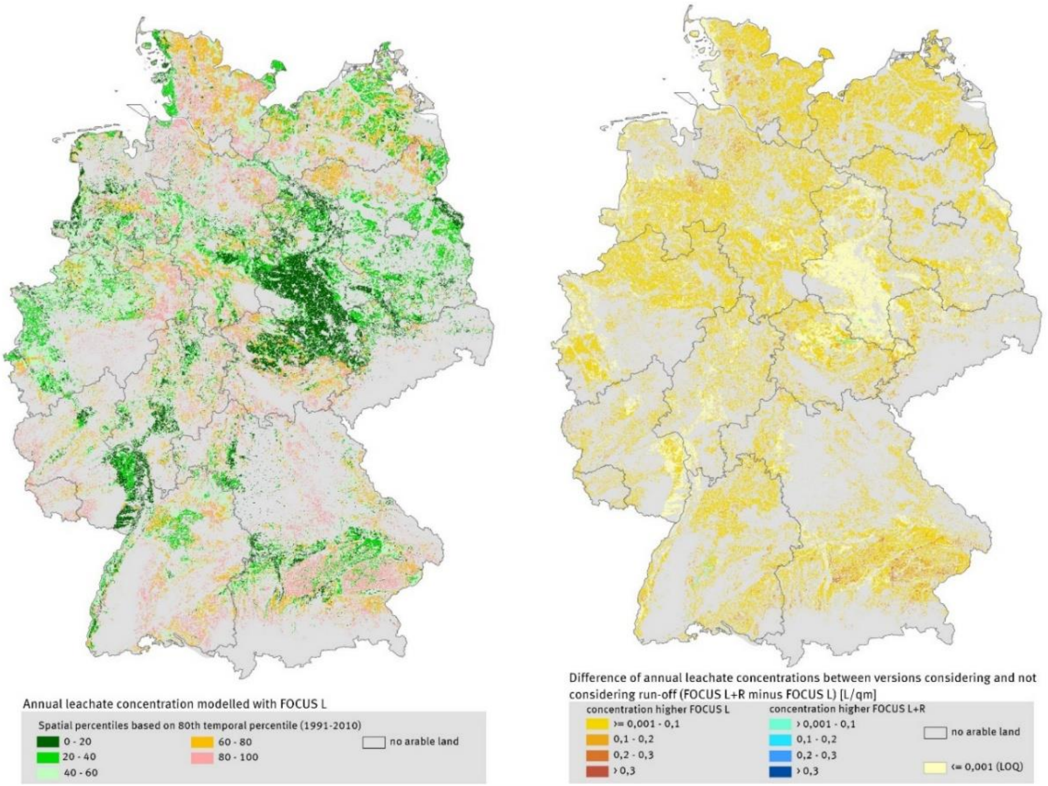
Figure 68 and Figure 69 illustrate that the spatial distribution of relative leachate concentrations calculated as percentiles and based on the FOCUS modelling approach (FOCUS L) is very similar between maize and winter cereals, although overall higher concentrations are calculated in winter cereals (see Table 51, Table 52). Higher concentrations in winter cereals are in line with modelling exercises based on scenarios provided in European Commission (2014). The reason is that applications in autumn usually lead to more conservative modelling results compared to spring and summer applications. This is because most of the percolate fluxes are expected to appear in autumn and winter, and the time for the pesticide being degraded in the upper soil horizon after application until the main groundwater recharge is shorter. Furthermore, the influence of runoff on the absolute percolate concentrations seems to be also quite comparable for both crops used in the model (Figure 68, Figure 69). In most of the agricultural areas the estimated leachate concentration is reduced by up to 0.1 µg/L due to runoff, and in some areas reduced by 0.1 to 0.2 µg/L. It is noticeable that even higher leachate concentrations up to 0.1 µg/L are calculated for the spring application in maize in a few areas by considering runoff.

Figure 68: **Influence of runoff on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in maize**



Source: own illustration, Fraunhofer IME.

Figure 69: **Influence of runoff on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in winter cereals**



Source: own illustration, Fraunhofer IME.

Comparing the spatial 80th percentile and spatial median of the percolate concentrations (Table 51, Table 52) demonstrates that runoff indeed influences the leaching results in the unsaturated soil zone. A reduction of leachate concentrations in a range of 10 % to 68 % refers to realistic worst-case situations represented by the 80th spatial and the 80th temporal percentile. For the spatial median and the 80th temporal percentile a comparable reduction between 10 % to 93 % was calculated. Obviously, the selection of the spatial percentile doesn't extremely influence the relative effect of the process runoff on the percolate concentrations. However, the effect is generally more pronounced in maize (spring application, e.g., 53 % for P2) than in winter cereals (autumn application, e.g., 12 % for P2) for all the dummy parent compounds with different degradation and sorption behaviour. When applied in spring, the effect of runoff is decreasing with increasing sorption and increasing persistence. The explanation would be that higher sorption generally leads to a reduction of compound concentrations in runoff and higher concentrations remain in the soil for leaching. For autumn applications the contrary was found. That could be well explained with the decreasing degradation rates from P1 to P3, so that significant substance amounts are still available for runoff in the following spring. This evaluation leads to the preliminary conclusion that the application time and crop is rather important on how runoff influences the modelled leaching concentration in 1 m soil depth. The compound properties are connected to this, but their influence might be rather smaller. This would need to be confirmed by modelling runs on a wider range of properties and application times.

Table 51: Influence of runoff on the 80th spatial percentiles of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L (no runoff) [µg/L]	FOCUS L+R (incl. runoff) [µg/L]	Reduction due to runoff [%]
Maize	P1	30	10	0.0222	0.0109	68
Maize	P2	60	20	0.0881	0.0510	53
Maize	P3	240	80	0.2049	0.1218	51
Winter cereals	P1	30	10	0.9295	0.8422	10
Winter cereals	P2	60	20	0.5681	0.5061	12
Winter cereals	P3	240	80	0.3794	0.3092	20

Table 52: Influence of runoff on the spatial median of annual leachate concentrations calculated with GeoPELMO DE

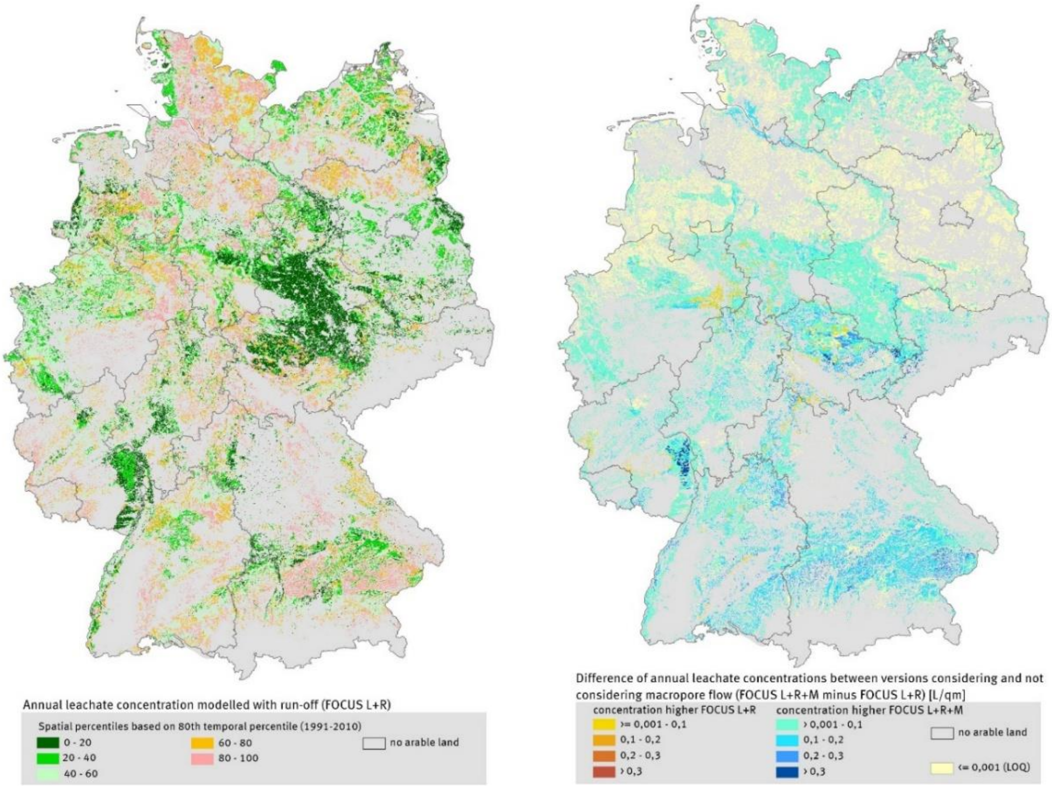
Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L (no runoff) [µg/L]	FOCUS L+R (incl. runoff) [µg/L]	Reduction due to runoff [%]
Maize	P1	30	10	0.0055	0.0020	93
Maize	P2	60	20	0.0196	0.0089	75
Maize	P3	240	80	0.0302	0.0143	72
Winter cereals	P1	30	10	0.2204	0.1990	10
Winter cereals	P2	60	20	0.1221	0.1003	20
Winter cereals	P3	240	80	0.0627	0.0489	25

Figure 70 and Figure 71 show the effect of macropore flow on the 80th temporal percentile of annual leachate concentrations in maize and winter cereals for the fictive active substance P2. The spatial patterns of the relative distribution of leachate concentrations are quite similar for both crops, when chromatographical flow and runoff (FOCUS L+R) are considered in GeoPELMO DE (maps on the left). Higher percentiles of modelled leachate concentrations occur generally in north-western Germany (i.e. in Schleswig-Holstein and Lower Saxony) as well as in central and southern Germany (i.e. in Bavaria). Larger areas with Schwarzerden (Phaeozems, Chernozems) or Braunerden (Cambisols, Brunic Arenosols) on silty loess deposits (i.e. in Saxony-Anhalt and Thuringia) are represented by lower percolate concentrations.

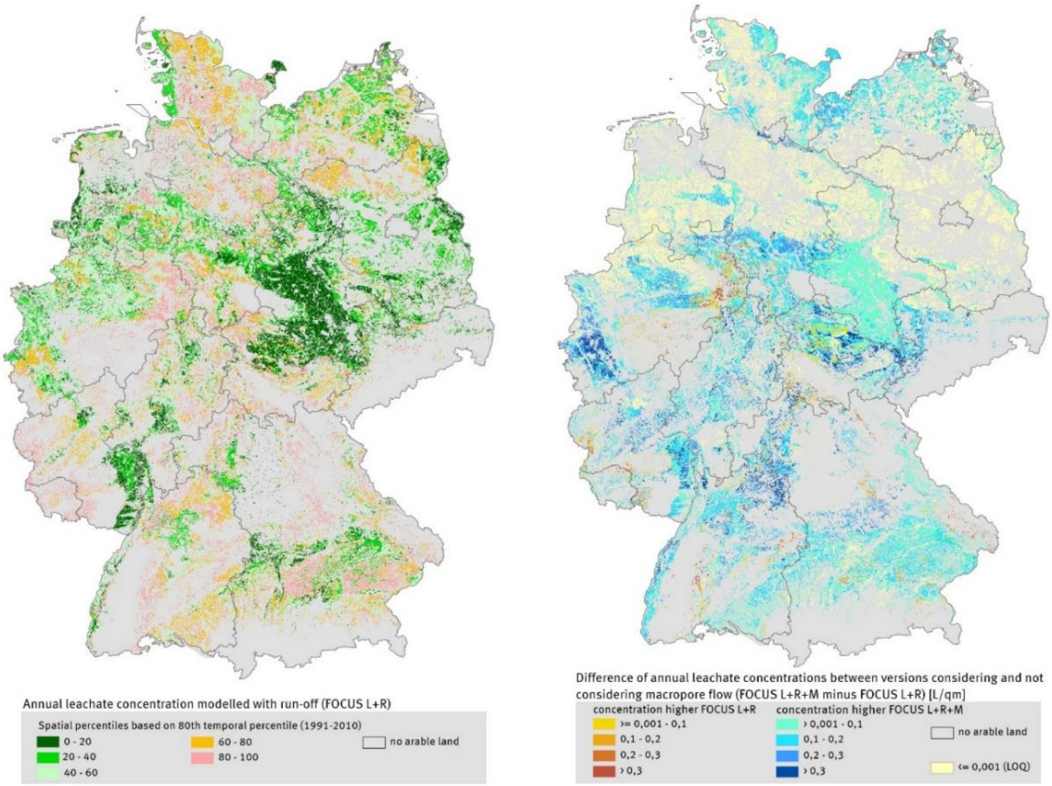
The maps on the right in clearly demonstrate that higher leachate concentrations are simulated in many regions when macropore flow is considered in GeoPELMO DE (FOCUS L+R+M) (Figure 70, Figure 71). Especially in central and southern Germany, the effect of macropore flow is dominant. Here, the differences in the forelands of the Harz mountains and in some parts of Bavaria are most prominent. The yellow colours mainly in Northern Germany represent the areas with sandy soil deposits where preferential flow is not implemented and only chromatographic flow and runoff are considered in GeoPELMO DE. A stronger increase of the absolute leachate concentration is visible in the maps for winter cereals. However, winter cereals are characterised by overall higher concentrations than maize and the relative differences are therefore comparatively smaller (see Table 53, Table 54).

Figure 70: **Influence of macropore flow on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in maize**



Source: own illustration, Fraunhofer IME.

Figure 71: **Influence of macropore flow on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in winter cereals**



Source: own illustration, Fraunhofer IME.

Comparing the spatial 80th percentile and the spatial median of the percolate concentrations based on the 80th temporal percentiles (Table 53, Table 54) demonstrates that macropore flow influences the leaching results more than runoff. The effect is generally more pronounced in maize (e.g., spring application, factor 5.1 for P1) than in winter cereals (e.g., autumn application, factor 1.1 for P1) for all three fictive active substances with different sorption and degradation properties. However, when applied in spring the effect of macropore flow is decreasing with increasing sorption. This same effect was also found for runoff. The explanation would be that higher sorption generally leads to a reduction of compound concentrations in the preferential flow itself. Like runoff the opposite was found for autumn applications. This could be explained by decreasing degradation rates from P1 to P3, so that considerable amounts of substance are still available in the upper soil layer for macropore flow in the following spring.

Comparing different spatial percentiles, the absolute median leachate concentrations are always lower than the 80th percentile concentrations (about a factor of 2.5). However, regarding the relative results the influence of macropore flow is relatively higher at the spatial medians than at the 80th percentiles. Factors between 1.7 and 12.5 are calculated to quantify the impact of macropore flow on median pesticide concentrations in the percolate at 1 m soil depth dependent on the crop and application time and compound properties. Factors between 1.1 and 5.1 are calculated to quantify the impact of macropore flow based on the 80th percentile leachate concentrations. Obviously, the selection of a certain spatial percentile is important for the quantification of the process macropore flow on nationwide percolate concentrations. Finally, the influence of macropore flow is decreasing with higher percentile selection for the three fictive active substances.

Table 53: Influence of macropore flow on the 80th spatial percentiles of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

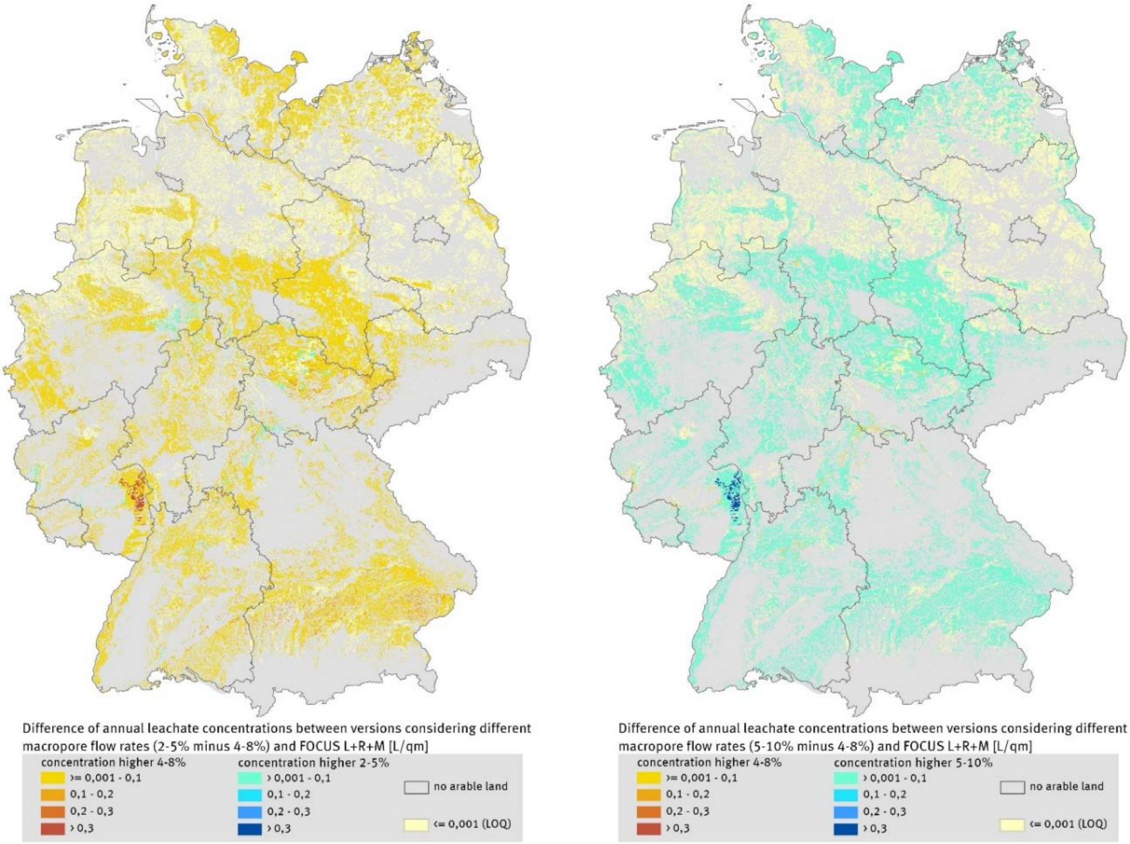
Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R (no macro-pore flow) [µg/L]	FOCUS L+R+M (incl. macro-pore flow) [µg/L]	Increase of concentration (ratio) [-]
Maize	P1	30	10	0.0109	0.0563	5.2
Maize	P2	60	20	0.0510	0.1464	2.9
Maize	P3	240	80	0.1218	0.2499	2.1
Winter cereals	P1	30	10	0.8422	0.9358	1.1
Winter cereals	P2	60	20	0.5061	0.6364	1.3
Winter cereals	P3	240	80	0.3092	0.4300	1.4

Table 54: Influence of macropore flow on the spatial median of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R (no macro-pore flow) [µg/L]	FOCUS L+R+M (incl. macro-pore flow) [µg/L]	Increase of concentration (ratio) [-]
Maize	P1	30	10	0.0020	0.0249	12.5
Maize	P2	60	20	0.0089	0.0691	7.8
Maize	P3	240	80	0.0143	0.1038	7.3
Winter cereals	P1	30	10	0.1990	0.3313	1.7
Winter cereals	P2	60	20	0.1003	0.2295	2.3
Winter cereals	P3	240	80	0.0489	0.1435	2.9

Figure 72: Influence of different macropore flow rates on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in maize



Source: own illustration, Fraunhofer IME.

To evaluate the sensitivity of the macropore flow parametrisation in GeoPELMO DE on the nationwide percolate concentrations in 1 m soil depth the three following different settings are additionally compared:

- low dynamic macropore flow: minimum fraction: 2 %, maximum fraction: 5 %
- standard dynamic macropore flow: minimum fraction: 4 %, maximum fraction: 8 %
- high dynamic macropore flow: minimum fraction: 5 %, maximum fraction: 10 %

The percentages above refer to the soil classes ‘high macropore flow’ (12.3 % of the agricultural area). For the soil class with ‘moderate macropore flow’ (52.9 % of the agricultural area) a reduction of 50 % for the minimum and the maximum fractions is always implemented in PELMO. No macropore flow and only chromatographic flow is considered for 34.8 % of the agricultural are in Germany (see chapters 4.3.2 and 4.3.5).

Figure 9 29 illustrates in two maps the nationwide differences of absolute percolate concentrations for the fictive substance P2 in maize when the standard dynamic macropore flow setting in GeoPELMO DE (4-8 %) is reduced to 2-5 % (on the left) or increased up to 5-10 % (on the right). As expected, reducing macropore flow mainly lowers the leachate concentrations and increasing the percentage of macropores flow leads to higher percolate concentrations. However, the effect is less pronounced when the parametrisation in the macropore flow module in GeoPELMO DE is changed compared to switching macropore flow on or off in total (see Figure 72).

A comparison of different percentiles for the different fictive compounds P1, P2, P3 in maize and winter cereals demonstrates that the impact of the different macropore flow parametrisations for leaching is limited for all three compounds. The results are furthermore in line with the previous finding that changing the macropore flow parametrisation is generally more sensitive in maize compared to winter cereals (Table 55, Table 56). And it is noticeable that the percentage differences in the percolate concentrations are higher between the two macropore flow parameterisations of 2-5 % and 4-8 % than between the parametrisations of 4-8 % and 5-10 %. Obviously, the selection of the spatial percentile has only a limited influence by comparing three different macropore flow parametrisation with resulting percolate concentrations.

Table 55: Influence of different macropore flow parametrisations on the 80th spatial percentiles of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	FOCUS L+R+M 2-5 % macropore flow [µg/L]	FOCUS L+R+M 4-8 % macropore flow [µg/L]	FOCUS L+R+M 5-10 % macropore flow [µg/L]	Increase between 4-8 % and 2-5 % [%]	Increase between 5-10 % and 4-8 % [%]
Maize	P1	0.0382	0.0563	0.0678	38	19
Maize	P2	0.1048	0.1464	0.1732	33	17
Maize	P3	0.2042	0.2619	0.2960	25	12
Winter cereals	P1	0.8681	0.9358	0.9758	8	4
Winter cereals	P2	0.5525	0.6364	0.7027	14	10
Winter cereals	P3	0.3699	0.4300	0.4682	15	9

Table 56: **Influence of different macropore flow parametrisations on the spatial medias of annual leachate concentrations calculated with GeoPELMO DE**

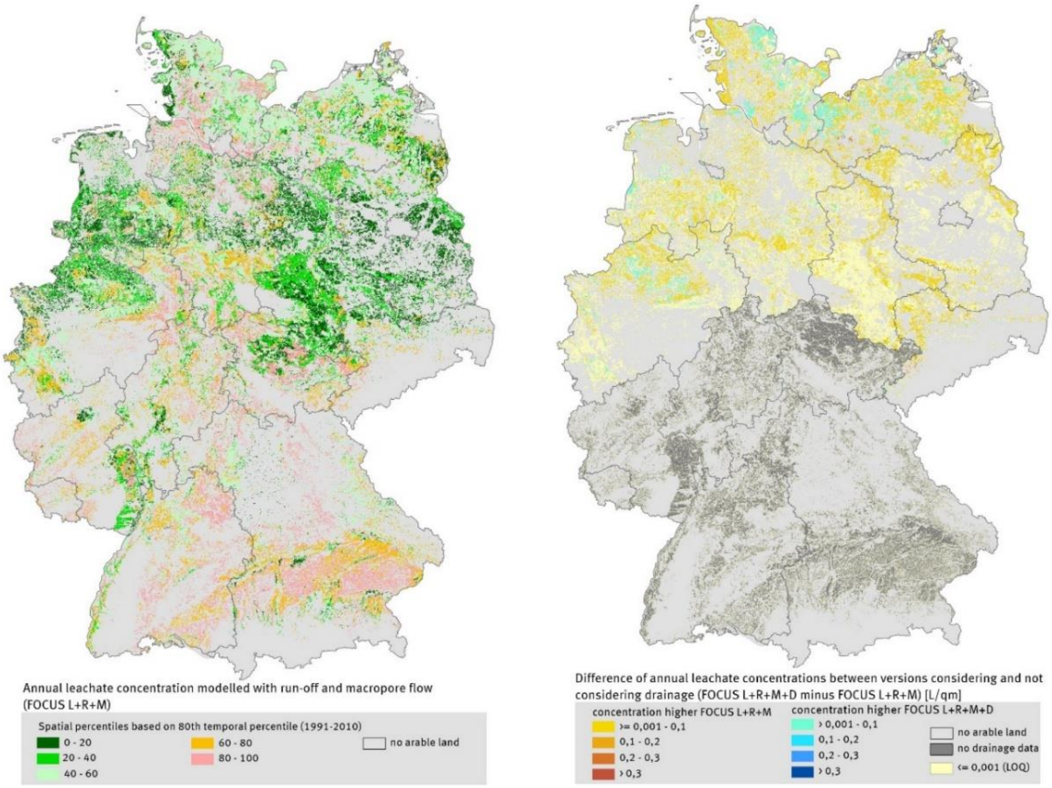
Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	FOCUS L+R+M 2-5 % macropore flow [µg/L]	FOCUS L+R+M 4-8 % macropore flow [µg/L]	FOCUS L+R+M 5-10 % macropore flow [µg/L]	Increase between 4-8 % and 2-5 % [%]	Increase between 5-10 % and 4-8 % [%]
Maize	P1	0.0165	0.0249	0.0297	41	18
Maize	P2	0.0448	0.0691	0.0845	43	20
Maize	P3	0.0744	0.1154	0.1428	43	21
Winter cereals	P1	0.2593	0.3313	0.3658	24	10
Winter cereals	P2	0.1714	0.2295	0.2572	29	11
Winter cereals	P3	0.0978	0.1435	0.1713	38	18

Artificial drainage via drainpipes was implemented in GeoPELMO DE based in the spatially distributed efficiency factor f_{eff} (see chapter 4.5.4.1). The factor causes reduced water fluxes below 80 cm soil depth in potentially drained agricultural fields. This increases the residence time of the applied pesticides below 80 cm, which means more time for degradation is available before a substance will reach the soil depth of 1 m. That will finally result in lower percolate concentrations at the bottom of the soil core.

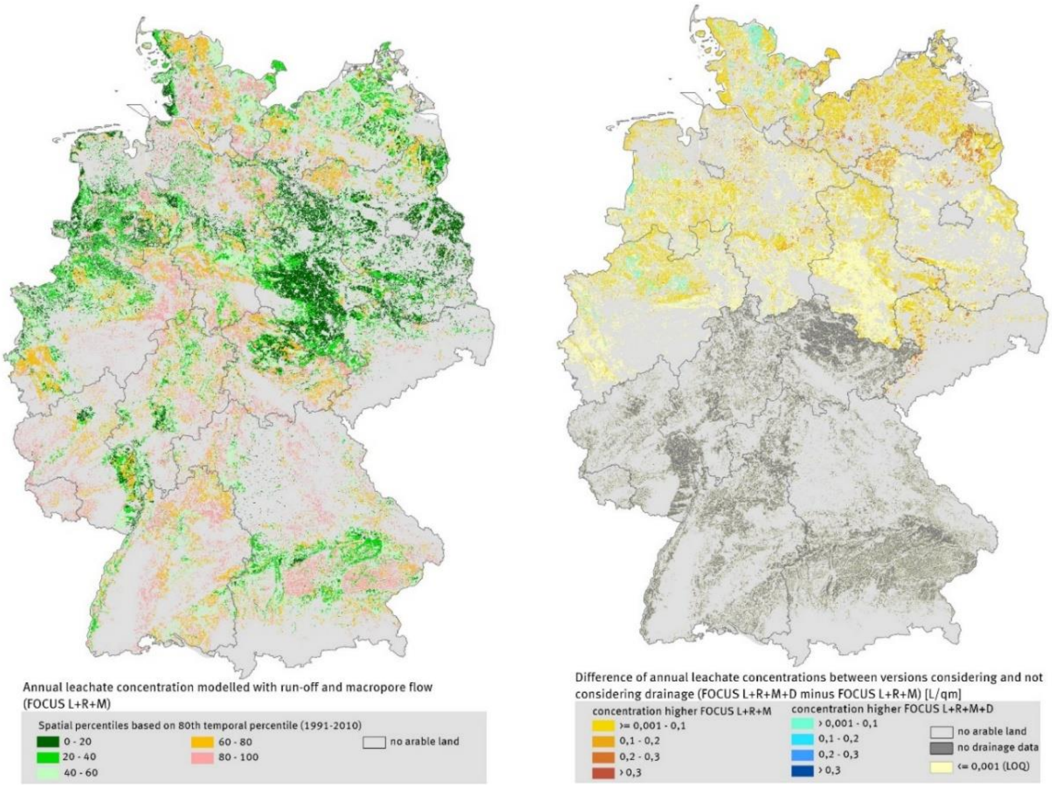
Figure 73 and Figure 74 illustrate that the spatial distribution of relative leachate concentrations calculated as percentiles (on the left) considering drainage beside runoff and macropore flow is different between maize and winter cereals. A comparison with the figures before provides evidence that drainage flow influences the percolate concentrations and their ranking in percentiles mainly in Northern Germany. This is caused by the fact that drainage was only considered in the northern federal states with unconsolidated rock deposits for which information on potential drained areas was available. Because percolate concentrations are not reduced nationwide but in selected regions only, this finally leads to a change of the spatial distribution of percentiles. However, the change of absolute percolate concentrations due to drainage is rather small for both crops as indicated by the right maps in Figure 73 and Figure 74. A reduction of less than 0.1 µ/L (or even no reduction) is visible in most agricultural areas. In few areas, a reduction of more than 0.1 µ/L can be observed. And even in a few areas, drainage leads to higher percolate concentrations as well. Overall, the absolute changes in winter cereals are higher than in maize, although higher percolate concentrations are also calculated in winter cereals, which tends to relativize this observation.

Figure 73: Influence of drainage on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in maize



Source: own illustration, Fraunhofer IME.

Figure 74: Influence of drainage on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in winter cereals



Source: own illustration, Fraunhofer IME.

Comparing the spatial 80th percentile and spatial median percolate concentration (Table 57, Table 58) demonstrates that drainage flow leads to a reduction of leaching. However, the calculated percentages show rather a small relative effect. A reduction of leachate concentrations due to drainage in a range of 1.0 % to 4.4 % refers to realistic worst-case situations represented by the 80th spatial and the 80th temporal percentile. For the spatial median and the 80th temporal percentile a reduction between 3.2 % to 10.9 % was calculated. Obviously, the selection of the spatial percentile has some influence of the process drainage flow on the percolate concentrations at 1 m soil depth. Furthermore, the consideration of drainage flow shows a stronger relative influence for the autumn application in winter cereals (e.g., a reduction of 4.4 %, 1.7 % and 3.7 % for P1, P2 and P3 when the 80th spatial percentile is compared) than for the spring application in maize (e.g., a reduction of 2.0 %, 1.0 % and 1.8 % for P1, P2 and P3), even if this difference is rather small (see Table 57).

Table 57: Influence of drainage flow on the 80th spatial percentiles of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R+M (no drainage) [µg/L]	FOCUS L+R+M+D (incl. drainage) [µg/L]	Reduction due to drainage [%]
Maize	P1	30	10	0.0563	0.0552	2.0
Maize	P2	60	20	0.1464	0.1450	1.0
Maize	P3	240	80	0.2619	0.2573	1.8
Winter cereals	P1	30	10	0.9358	0.8957	4.4
Winter cereals	P2	60	20	0.6364	0.6255	1.7
Winter cereals	P3	240	80	0.4300	0.4143	3.7

Table 58: Influence of drainage flow on the spatial medians of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R+M (no drainage) [µg/L]	FOCUS L+R+M+D (incl. drainage) [µg/L]	Reduction due to drainage [%]
Maize	P1	30	10	0.0249	0.0230	7.9
Maize	P2	60	20	0.0691	0.0661	4.4
Maize	P3	240	80	0.1154	0.1118	3.2
Winter cereals	P1	30	10	0.3313	0.2970	10.9
Winter cereals	P2	60	20	0.2295	0.2087	9.5
Winter cereals	P3	240	80	0.1435	0.1383	3.7

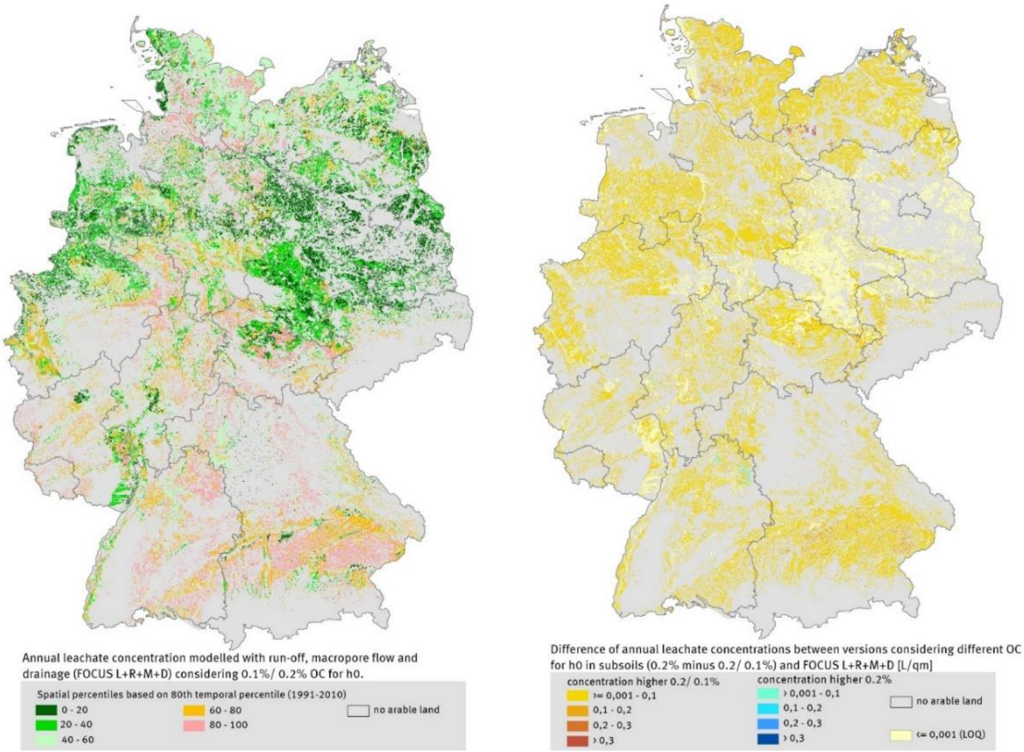
Comparable results are found when the spatial medians are compared (see Table 58). This result is different from runoff and macropore flow. Both processes had a stronger influence in the spring application in maize. The influence of drainage seems to be more pronounced for more mobile and faster degrading substances. This trend was also found when runoff and macropore flow were included in the simulation. However, the influence of substance properties on drainage is rather limited in the presented results and additional simulations would need to confirm those findings.

In section 4.2.1.2, an analysis was presented about the distribution of measured organic carbon contents for the organic matter class h0 in German subsoils. The evaluation was based on measured values from the permanent soil-monitoring program of the German federal states. Different options were discussed for the definition of the organic carbon content for the humus class h0 in the available geodata. Finally, it was decided to use a C_{org}-content value of 0.2 % for the humus class h0 in the soil depth 0 – 60 cm and 0.1 % for the humus class h0 in the soil depth 60 cm – 100 cm. This parameter setting was used for all simulations with GeoPELMO DE presented so far. However, to check the sensitivity of the organic carbon content default values in subsoils for the nationwide estimation of percolate concentrations, additional PELMO simulations were performed with a less conservative organic carbon default content of 0.2 % for all h0-values in the geodata independent on their soil depth.

Figure 75 and Figure 76 illustrate the effect of replacing the soil humus class h0 in the German soil database from the BÜK200 (BGR 2018a) with different organic carbon content default values for estimation nationwide percolate concentrations of P2 in maize and winter cereals. The difference maps in both figures on the right clearly show that the humus class h0 is widespread in the profiles of the agricultural soils in the BÜK200, whereby the replacement with default values has a far-reaching spatial effect. Only larger areas in Saxony-Anhalt and Brandenburg are excluded from this effect. Finally, the use of higher default organic carbon values clearly leads to a reduction of the percolate concentrations at 1 m soil depth in most areas. In addition, the absolute changes in percolate concentrations due to different default organic carbon contents are higher in winter cereals than in maize. However, it must be considered that the calculated concentrations in the winter cereals are also significantly higher than in maize. The calculated percentages in Table 59 and Table 60 show that the relative changes in maize and winter cereals are nearly the same. That means that the influence on application time and crops seems to be rather limited.

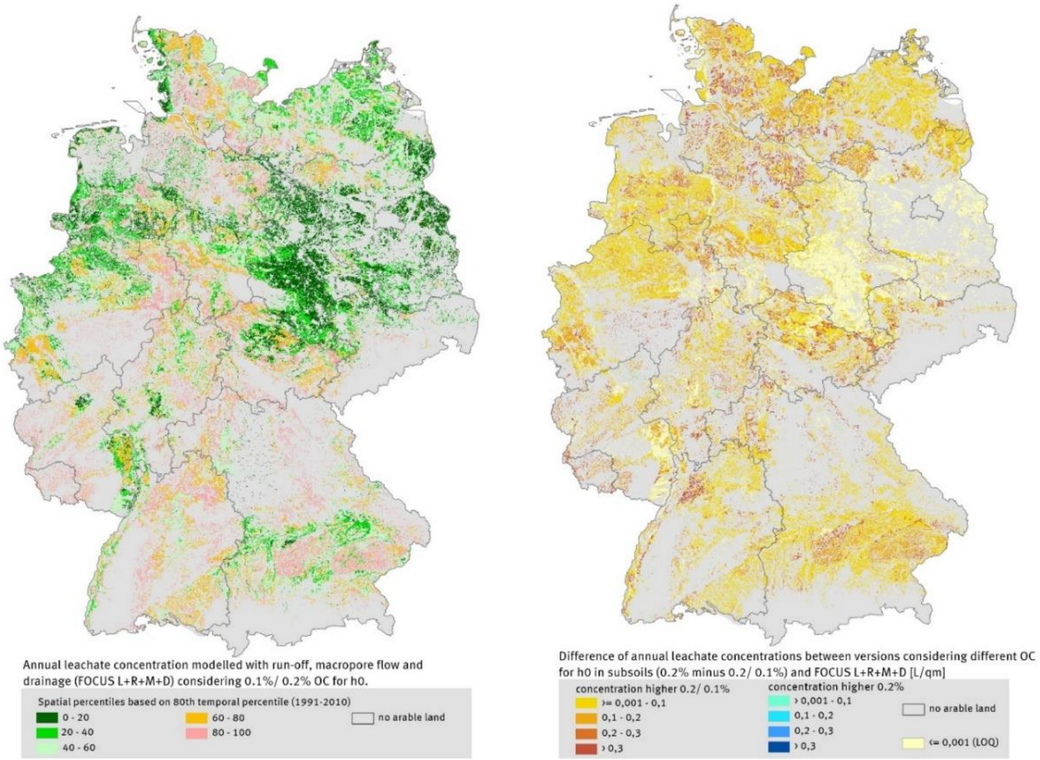
Comparing the spatial 80th percentile and spatial median percolate concentration (Table 59, Table 60) demonstrates that a default value of 0.2 % organic carbon for humus class h0 independent on the soil depth instead of taking 0.1 % and 0.2 % for different depth leads to a significant reduction of annual leachate concentrations. In particular, the relatively small change in organic carbon contents in the upper soil layers leads to a constant and significant change in the leachate concentrations. Referring to a realistic worst-case situation by combining the 80th spatial and the 80th temporal percentile, a reduction of percolate concentrations between 22 % and 36 % are calculated when higher organic carbon content values are taken as default values for humus class h0. Referring to a spatial situation by combining the spatial median and the 80th temporal percentile, a reduction of percolate concentrations between 25 % and 49 % are calculated. Obviously, the selection of the spatial percentile has a minor impact on the sensitivity of organic carbon parametrisation on the percolate concentrations at 1 m soil depth, whereby the impact is a bit higher when calculating the spatial median. The results show that

Figure 75: **Influence of different default organic carbon contents for humus class h0 in subsoils on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in maize**



Source: own illustration, Fraunhofer IME.

Figure 76: **Influence of different default organic carbon contents for humus class h0 in subsoils on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in winter cereals**



Source: own illustration, Fraunhofer IME.

organic carbon content parametrisation for humus class h0 has no different effects on the crop and application timing. Comparing substance properties, there is a slightly higher sensitivity for substances with better sorption and lower degradation (P3).

Table 59: Influence of different default organic carbon contents for humus class h0 in subsoils on the 80th spatial percentiles of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R+M+D 0.1/0.2 % OC content for h0 (standard) [µg/L]	FOCUS L+R+M+D 0.2 % OC content for h0 [µg/L]	Reduction due to higher OC contents [%]
Maize	P1	30	10	0.0552	0.0444	22
Maize	P2	60	20	0.1450	0.1095	28
Maize	P3	240	80	0.2573	0.1787	36
Winter cereals	P1	30	10	0.8957	0.6890	26
Winter cereals	P2	60	20	0.6255	0.4890	25
Winter cereals	P3	240	80	0.4143	0.2988	32

Table 60: Influence of different default organic carbon contents for humus class h0 in subsoils on the spatial medians of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R+M+D 0.1/0.2 % OC content for h0 (standard) [µg/L]	FOCUS L+R+M+D 0.2 % OC content for h0 [µg/L]	Reduction due to higher OC contents [%]
Maize	P1	30	10	0.0230	0.0178	25
Maize	P2	60	20	0.0661	0.0457	36
Maize	P3	240	80	0.1118	0.0657	52
Winter cereals	P1	30	10	0.2970	0.2290	26
Winter cereals	P2	60	20	0.2087	0.1418	38
Winter cereals	P3	240	80	0.1383	0.0842	49

5.4.1.1 Summary for active substances percolate concentrations

The results of the analyses in this chapter finally show that the soil water balance processes like runoff, chromatographic flow, preferential flow, drainage flow and their parameterisation, the substance properties sorption and degradation as well as different application times and crops have an influence on the modelling of nationwide pesticide leaching concentrations for parent compounds, some of them not in the same direction. The choice of spatial and temporal percentiles also plays a role and does not always show the same influence of individual parameters. That makes it finally difficult to forecast the influence of each single process and parameter for nationwide spatially distributed leaching modelling results with a model like GeoPELMO DE.

There is evidence that runoff and drainage mainly lead to reduced leachate concentrations for active substances in the unsaturated soil zone, while macropore flow leads in general to higher concentrations. The impact of macropore flow itself was higher than different parametrisations of macropore flow. Considering different crops and application times, the relative effect of runoff and macropore flow was shown to be higher for spring application in maize compared to autumn application in winter cereals, whereby both processes influence the leaching behaviour in opposite directions. The influence of drainage is rather limited, and differences are minor between both crops and between different application times. Since seasonal effects for drainage flow have been shown before, the influence of drainage on the leaching behaviour in winter cereals might be slightly higher. The added influence of all three additional processes on the nationwide percolate concentrations for three fictive active substances is finally provided in Table 61 and Table 62. The ratio of the leaching results from both modelling runs (FOCUS L and FOCUS L+R+M+D) provides evidence that in most cases higher spatial median and spatial 80th percentile percolate concentrations are estimated for active substances, if runoff, macropore flow and drainage are additionally considered in the modelling routine. The ratios of concentrations show the increasing trend in a range between 1.1 and 4.18. For one situation (P1 as mobile, fast degrading substance in winter cereals) lower leachate concentrations with a ratio of 0.96 are calculated.

In addition, the spatial modelling results are very sensitive to organic carbon contents in soil. It was shown that replacing the humus class h0 with slightly different default organic carbon contents leads to comparable high changes in leachate concentrations for parent compounds rather independent from individual crops, application timings and the spatial percentile selection. That gives good reasons to look for reliable parametrisations of organic carbon contents based on measured values.

The spatial influence of model results considering all three processes runoff, macropore flow and drainage (FOCUS L+R+M+D) in addition to the FOCUS leaching approach (FOCUS L) is provided for dummy active substance P2 in different maps in Figure 77 and Figure 78. The comparison analysis show that predicted leachate concentrations based on the FOCUS modelling routine are mainly higher in the northern belt in Germany with glacial deposits and sandy soils. Increasing concentrations are predicted in large parts in central and southern Germany if runoff, macropore flow and drainage are additionally considered in the modelling. The comparison shows that the relative vulnerability class can easily change in large areas and on a landscape scale level for both crops, maize and winter cereals, if runoff, macropore flow and drainage are considered.

Table 61: Combined influence of runoff, macropore flow and drainage on the spatial 80th percentile of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops. The calculated ratio represents the increase of leachate concentrations due to the consideration of runoff, macropore flow and drainage. The results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

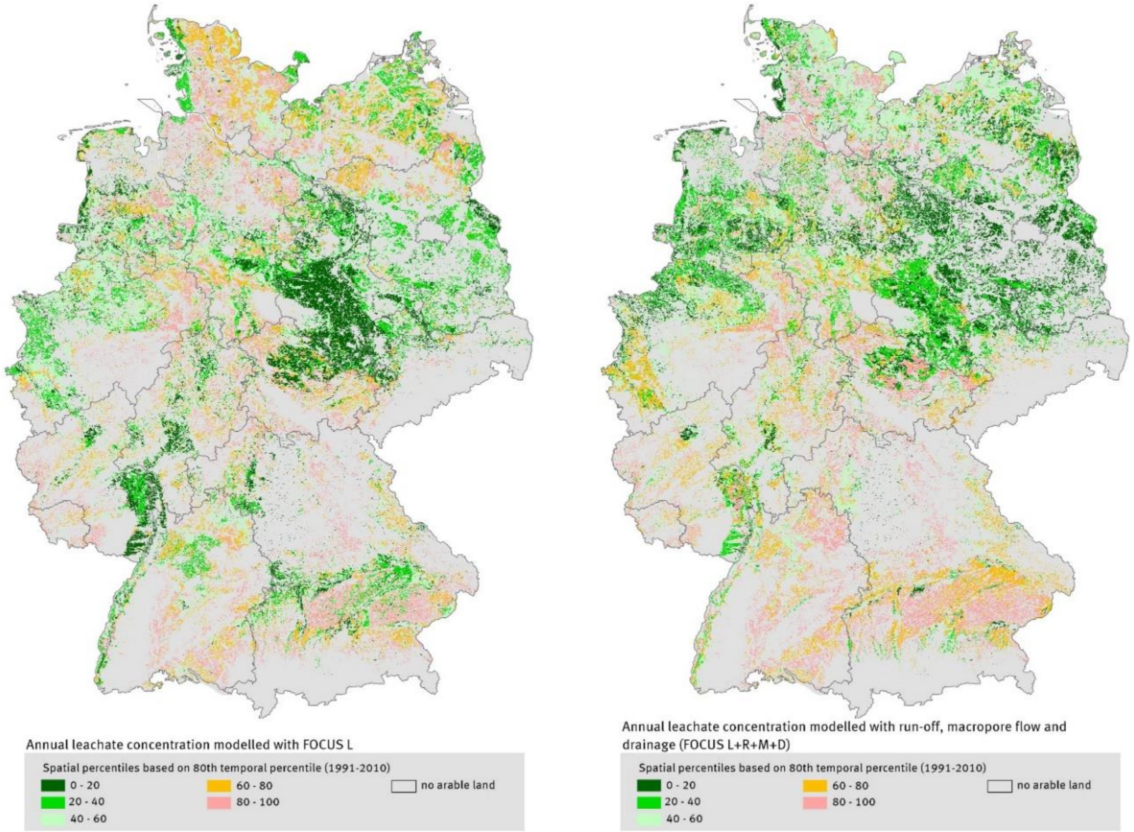
Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L [µg/L]	FOCUS L+R+M+D [µg/L]	Increasing leachate concentrations (ratio) [-]
Maize	P1	30	10	0.0222	0.0552	2.49
Maize	P2	60	20	0.0881	0.1450	1.65
Maize	P3	240	80	0.2049	0.2573	1.26
Winter cereals	P1	30	10	0.9295	0.8957	0.96
Winter cereals	P2	60	20	0.5681	0.6255	1.10
Winter cereals	P3	240	80	0.3794	0.4143	1.09

Table 62: Combined influence of runoff, macropore flow and drainage on the spatial median of annual leachate concentrations calculated with GeoPELMO DE

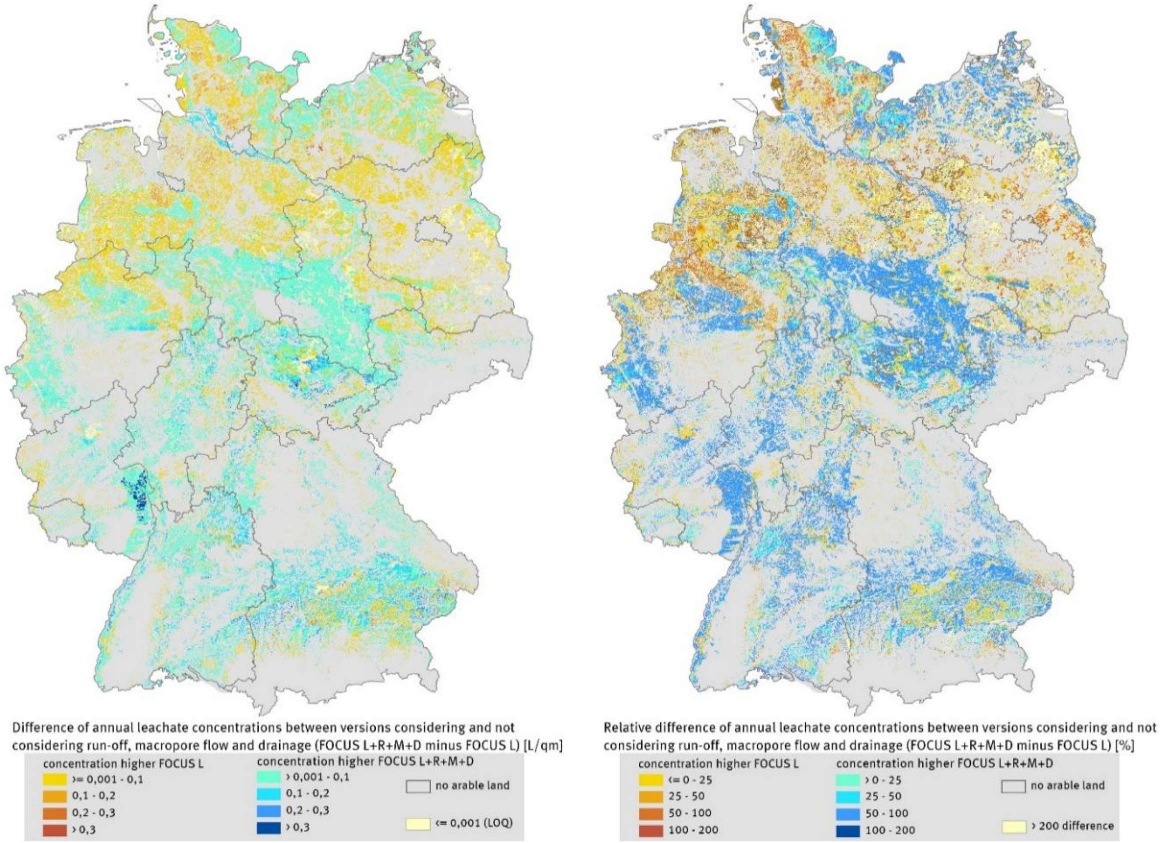
Model simulations are conducted for three dummy active substances and two crops. The calculated ratio represents the increase of leachate concentrations due to the consideration of runoff, macropore flow and drainage. The results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L [µg/L]	FOCUS L+R+M+D [µg/L]	Increasing leachate concentrations (ratio) [-]
Maize	P1	30	10	0.0055	0.0230	4.18
Maize	P2	60	20	0.0196	0.0661	3.37
Maize	P3	240	80	0.0302	0.1118	3.70
Winter cereals	P1	30	10	0.2204	0.2970	1.35
Winter cereals	P2	60	20	0.1221	0.2087	1.71
Winter cereals	P3	240	80	0.0627	0.1383	2.21

Figure 77: Combined influence of runoff, macropore flow and drainage on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in maize


Annual leachate concentration modelled with FOCUS L

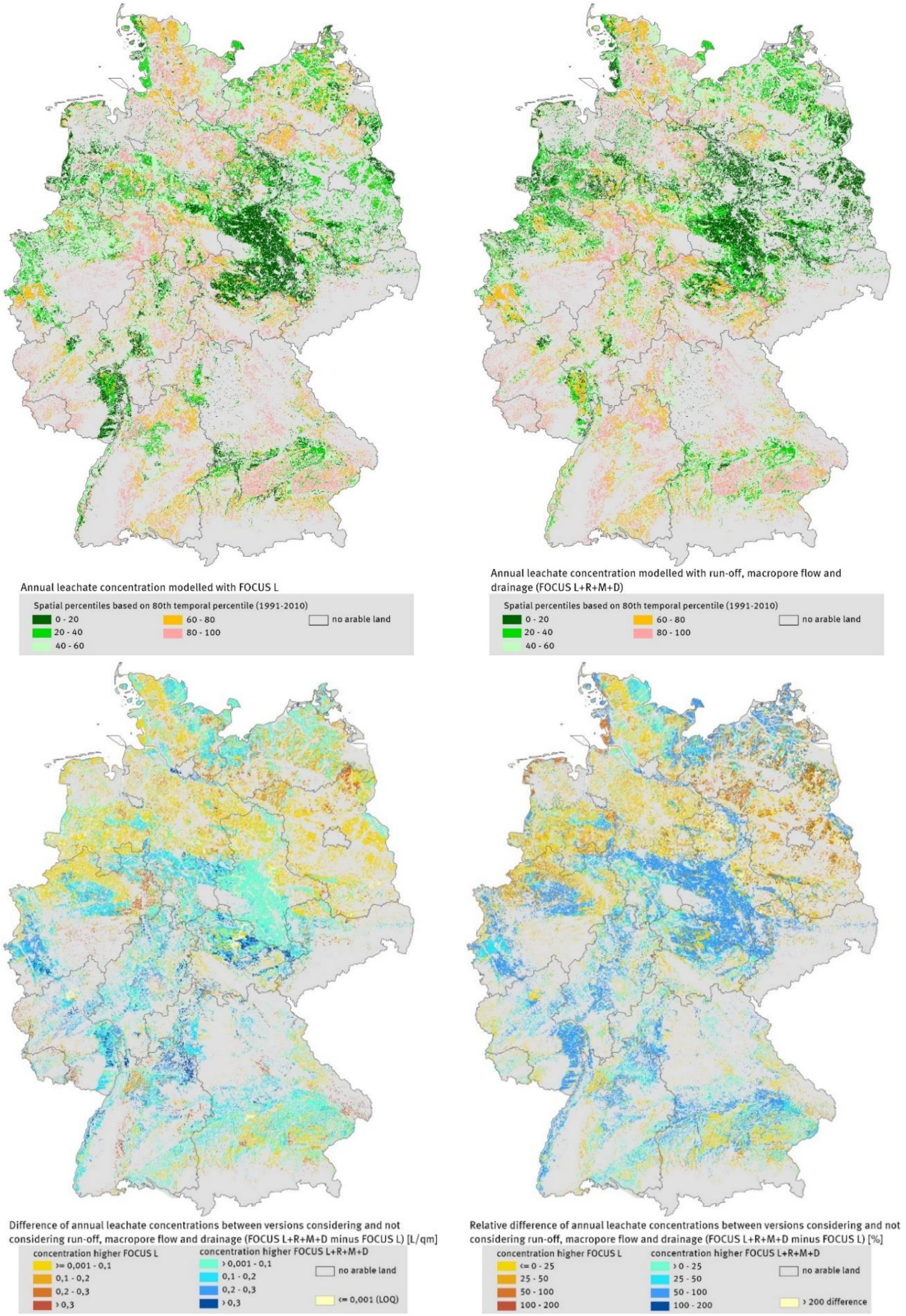
Annual leachate concentration modelled with run-off, macropore flow and drainage (FOCUS L+R+M+D)


Difference of annual leachate concentrations between versions considering and not considering run-off, macropore flow and drainage (FOCUS L+R+M+D minus FOCUS L) [L/qm]

Relative difference of annual leachate concentrations between versions considering and not considering run-off, macropore flow and drainage (FOCUS L+R+M+D minus FOCUS L) [%]

Source: own illustration, Fraunhofer IME.

Figure 78: **Combined influence of runoff, macropore flow and drainage on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy active substance P2 in winter cereals**



Source: own illustration, Fraunhofer IME.

5.4.2 Metabolites

Nationwide average annual percolate concentrations are calculated and evaluated for two fictive metabolites (M1, M2) with different degradation and sorption behaviour which are formed with different rates from different fictive parent compounds P1, P2 and P3 (see section 5.1).

The tables in this chapter contain statistical values such as the median and 80th percentile of the spatially varying leachate concentrations for both metabolites M1 and M2. Modelled concentrations are compared in terms of evaluating the influence of the modelling routines for each new process like runoff, macropore flow and drainage. In addition, the influence of different default values for organic carbon contents in subsoils with humus class 0 is analysed. In the summary section of this chapter the impact of all new process like runoff, macropore flow and drainage to predict leachate concentrations is evaluated. Maps are provided as example for the dummy metabolite M1 (very mobile & moderately persistent) formed with 50 % of formation from dummy active substance P2 (moderately mobile and fast degrading). The aim is to visualise the spatial effect of the additional processes like runoff, macropore flow and artificial drainage flow in Germany (see Figure 79).

Comparing the spatial 80th percentile and spatial median of the percolate concentrations (Table 63 and Table 64) demonstrates that the influence of runoff on metabolite concentrations in the percolate in 1 soil depth is much smaller than for the parent compounds. The relative change of the leachate concentration due to runoff is a little bit higher in maize (spring application, e.g., -6.7% for M2 when formed by P1) than in winter cereals (autumn application, e.g., 2.5% for M2 when formed by P1). Including runoff in the simulations can lead to a decrease or increase of the percolate concentrations for metabolites. Increasing leachate concentrations for metabolites were found when the parent compound was applied in autumn (crop: winter cereals) and decreasing leachate concentrations were found when the parent compound was applied in spring (crop: maize). This could be the effect of two contrary processes. Including runoff may reduce the active substance on the soil surface and therefore the formation of the metabolite in the soil, followed by reduction of percolate concentrations. At the same time, it may reduce the amount of percolate water which could slightly increase the respective percolate concentrations for metabolites. In any case, the effect is very small, and it can be concluded that runoff only slightly changes the estimated leachate concentrations for metabolites.

The influence of macropore flow on the spatial 80th percentile and the spatial median of the percolate concentration for primary dummy metabolites in 1 m soil depth is provided in Table 65 and Table 66. Compared to active substances the effect of macropore flow on estimated metabolite concentrations in the percolate is very low and amounts to approximately 1 %. It depends on the formation fraction and properties. Furthermore, including macropore flow in the simulations can lead to slightly increasing or decreasing percolate concentrations for the metabolites. Increasing concentrations were mainly found when the parent compound was applied in spring (crop: maize), and decreasing concentrations were mainly found when the parent compound was applied in autumn (crop: winter cereals). The reasoning behind this second effect could be a reduced formation of the metabolites because a certain amount of active substance has been already fast transported though the soil profile by macropore flow. In any case, the effect of macropore flow for the leaching of metabolites is only very small and seems to be negligible. A selection of the spatial 80th percentile or the median hardly changes the results.

Table 63: Influence of runoff on the 80th spatial percentiles of annual metabolite leachate concentrations with GeoPELMO DE

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010)

Crop	Metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L (no runoff) [µg/L]	FOCUS L+R (incl. runoff) [µg/L]	Difference due to runoff [%]
Maize	M2 (P1)	30	80	10.749	10.052	-6.7
Maize	M1 (P2)	10	40	4.873	4.811	-1.3
Maize	M2 (P2)	30	80	5.968	5.605	-6.3
Maize	M2 (P3)	30	80	14.674	14.193	-3.3
Winter cereals	M2 (P1)	30	80	19.954	20.451	2.5
Winter cereals	M1 (P2)	10	40	7.261	7.383	1.7
Winter cereals	M2 (P2)	30	80	8.794	8.948	1.7
Winter cereals	M2 (P3)	30	80	16.537	16.564	0.2

Table 64: Influence of runoff on the spatial median of annual metabolite leachate concentrations with GeoPELMO DE

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010)

Crop	Metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L (no runoff) [µg/L]	FOCUS L+R (incl. runoff) [µg/L]	Difference due to runoff [%]
Maize	M2 (P1)	30	80	8.245	7.673	-7.2
Maize	M1 (P2)	10	40	3.561	3.277	-8.3
Maize	M2 (P2)	30	80	4.373	4.117	-6.0
Maize	M2 (P3)	30	80	10.405	10.035	-3.6
Winter cereals	M2 (P1)	30	80	13.587	13.840	1.8
Winter cereals	M1 (P2)	10	40	5.212	5.273	1.2
Winter cereals	M2 (P2)	30	80	5.864	5.908	0.7
Winter cereals	M2 (P3)	30	80	11.103	10.996	-1.0

Table 65: Influence of macropore flow on the 80th spatial percentiles of annual metabolite leachate concentrations with GeoPELMO DE

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010)

Crop	Metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R (no macro-pore flow) [µg/L]	FOCUS L+R+M (incl. macro-pore flow) [µg/L]	Difference due to macropore flow [%]
Maize	M2 (P1)	30	80	10.052	10.179	1.3
Maize	M1 (P2)	10	40	4.811	4.790	-0.4
Maize	M2 (P2)	30	80	5.605	5.644	0.7
Maize	M2 (P3)	30	80	14.193	14.205	0.1
Winter cereals	M2 (P1)	30	80	20.451	20.274	-0.9
Winter cereals	M1 (P2)	10	40	7.383	7.331	-0.7
Winter cereals	M2 (P2)	30	80	8.948	8.845	-1.2
Winter cereals	M2 (P3)	30	80	16.564	16.438	-0.8

Table 66: Influence of macropore flow on the spatial median of annual metabolite leachate concentrations with GeoPELMO DE

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010)

Crop	Metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R (no macro-pore flow) [µg/L]	FOCUS L+R+M (incl. macro-pore flow) [µg/L]	Difference due to macropore flow [%]
Maize	M2 (P1)	30	80	7.673	7.732	0.8
Maize	M1 (P2)	10	40	3.277	3.304	0.8
Maize	M2 (P2)	30	80	4.117	4.142	0.6
Maize	M2 (P3)	30	80	10.035	9.778	-2.6
Winter cereals	M2 (P1)	30	80	13.840	13.701	-1.0
Winter cereals	M1 (P2)	10	40	5.273	5.208	-1.2
Winter cereals	M2 (P2)	30	80	5.908	5.823	-1.4
Winter cereals	M2 (P3)	30	80	10.996	10.888	-1.0

The influence of drainage flow on the spatial 80th percentiles and the spatial median of the percolate concentration for two dummy metabolites in 1 m soil depth is summarised in Table 67 and Table 68. The relative impact of drainage on metabolite concentrations in the percolate is rather low and quite comparable to the influence on percolate concentrations for the active substances (see section 5.4.1). An influence between -1.7 % and 2.6 % was calculated for the metabolite leaching referring to the 80th spatial and 80th temporal percentile and different crops (application time), formation fractions and active substance and metabolite properties (Table 67). Referring to the spatial median and 80th temporal percentile, the percolate concentration of the metabolites changes due to drainage in a range between -3.5 % and 2.3 % (Table 68). Including drainage in the simulations can lead to decreasing or increasing percolate concentrations for metabolites, whereby no regularities can be observed in each case. This is different compared to the observations for the active substances, where percolate concentrations have been always reduced due to drainage. Anyway, the relative effect of drainage on metabolite leaching seems rather low.

Table 67: Influence of drainage on the 80th spatial percentiles of annual metabolite leachate concentrations calculated with GeoPLELMO DE

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010)

Crop	Metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R+M (no drainage) [µg/L]	FOCUS L+R+M+D (incl. drainage) [µg/L]	Difference due to drainage [%]
Maize	M2 (P1)	30	80	10.179	10.341	1.6
Maize	M1 (P2)	10	40	4.790	4.790	0
Maize	M2 (P2)	30	80	5.644	5.648	0.1
Maize	M2 (P3)	30	80	14.205	13.962	-1.7
Winter cereals	M2 (P1)	30	80	20.274	20.112	-0.8
Winter cereals	M1 (P2)	10	40	7.331	7.525	2.6
Winter cereals	M2 (P2)	30	80	8.845	8.784	-0.7
Winter cereals	M2 (P3)	30	80	16.438	16.387	-0.3

Table 68: Influence of drainage on the spatial median of annual metabolite leachate concentrations with GeoPELMO DE

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010)

Crop	Metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R+M (no drainage) [µg/L]	FOCUS L+R+M+D (incl. drainage) [µg/L]	Difference due to drainage [%]
Maize	M2 (P1)	30	80	7.732	7.645	-1.1
Maize	M1 (P2)	10	40	3.304	3.190	-3.5
Maize	M2 (P2)	30	80	4.142	4.104	-0.9
Maize	M2 (P3)	30	80	9.778	9.971	2.0
Winter cereals	M2 (P1)	30	80	13.701	13.891	1.4
Winter cereals	M1 (P2)	10	40	5.208	5.133	-1.5
Winter cereals	M2 (P2)	30	80	5.823	5.942	2.0
Winter cereals	M2 (P3)	30	80	10.888	11.138	2.3

In section 4.2.2 an analysis was presented about the distribution of organic carbon contents for the organic matter class h0 in German subsoils. The evaluation was based on measured values from the permanent soil-monitoring program of the German federal states. Different options were discussed for the definition of the organic carbon content for the humus class h0 in the available geodata. Finally, it was decided to use a C_{org}-content value of 0.2 % for the humus class h0 in the soil depth 0 – 60 cm and 0.1 % for the humus class h0 in the soil depth 60 cm – 100 cm. This parameter setting was used for all simulations with GeoPELMO DE presented so far. However, to check the sensitivity of the organic carbon content default values in subsoils for the nationwide estimation of percolate concentrations, additional PELMO simulations were performed with a less conservative organic carbon default content of 0.2 % for all h0-values in the geodata independent on their soil depth.

Comparing the spatial 80th percentile and spatial median percolate concentration (Table 69 and Table 70) demonstrates that a default value of 0.2 % organic carbon for humus class h0 independent on the soil depth instead of taking 0.1 % and 0.2 % for different depth leads to a reduction of annual leachate concentrations for the metabolites. Compared to the leaching behaviour of the active substances (see section 5.4.1) the impact of the organic carbon parametrisation on metabolite concentrations in the percolate is significantly lower. Referring to a realistic worst-case situation by combining the 80th spatial and 80th temporal percentile, a reduction of the metabolite percolate concentrations between 2.4 % and 4.7 % are calculated when higher organic carbon content values are taken as default values for humus class h0 (Table 69). Referring to a spatial situation by combining the spatial median and the 80th temporal percentile, a reduction of percolate concentrations between 2.6 % and 4.9 % are calculated (Table 70). Obviously, the selection of the spatial percentile has a minor influence of the sensitivity of organic carbon parametrisation on the percolate concentrations at 1 m soil depth. There is no seasonal effect and no difference whether the substance was applied in spring (maize) or autumn (winter cereals). Comparing metabolite properties, there is a slightly higher sensitivity for the metabolite M2 with better sorption and slower degradation.

Table 69: **Influence of different default organic carbon contents for humus class h0 in subsoils on the 80th spatial percentiles of annual metabolite leachate concentrations calculated with GeoPELMO DE**

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010). All additional processes have been considered.

Crop	Metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R+M+D 0.1/0.2% OC content for h0 (standard) [µg/L]	FOCUS L+R+M+D 0.2% OC content for h0 [µg/L]	Reduction due to higher OC contents [%]
Maize	M2 (P1)	30	80	10.341	9.867	-4.7
Maize	M1 (P2)	10	40	4.790	4.676	-2.4
Maize	M2 (P2)	30	80	5.648	5.413	-4.2
Maize	M2 (P3)	30	80	13.962	13.425	-3.9
Winter cereals	M2 (P1)	30	80	20.112	19.475	-3.2
Winter cereals	M1 (P2)	10	40	7.525	7.311	-2.9
Winter cereals	M2 (P2)	30	80	8.784	8.533	-2.9
Winter cereals	M2 (P3)	30	80	16.387	15.783	-3.8

Table 70: **Influence of different default organic carbon contents for humus class h0 in subsoils on the spatial median of annual metabolite leachate concentrations calculated with GeoPELMO DE**

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different active substances and two crops based on the 80th temporal percentiles from 20 weather years (1991-2010). All additional processes have been considered.

Crop	Metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L+R+M+D 0.1/0.2% OC content for h0 (standard) [µg/L]	FOCUS L+R+M+D 0.2% OC content for h0 [µg/L]	Reduction due to higher OC contents [%]
Maize	M2 (P1)	30	80	7.645	7.277	-4.9
Maize	M1 (P2)	10	40	3.190	3.095	-3.0
Maize	M2 (P2)	30	80	4.104	3.908	-4.9
Maize	M2 (P3)	30	80	9.971	9.574	-4.1
Winter cereals	M2 (P1)	30	80	13.891	13.310	-4.3
Winter cereals	M1 (P2)	10	40	5.133	5.003	-2.6
Winter cereals	M2 (P2)	30	80	5.942	5.698	-4.2
Winter cereals	M2 (P3)	30	80	11.138	10.707	-3.9

5.4.2.1 Summary for metabolite percolate concentrations

The results of the analyses in this chapter finally show that soil water processes like runoff, chromatographic flow, preferential flow and drainage flow, the active substance and metabolite properties sorption and degradation as well as different application times and crops have an influence on the modelling of nationwide leaching concentrations for metabolites. However, it can be observed that the influence of those processes and parameters on the leaching estimated for metabolites are significantly lower compared to the active substances. The choice of spatial and temporal percentile also plays a minor role. That makes it difficult to forecast the influence of each single process and parameter for nationwide spatially distributed leaching modelling results for metabolites with a model like GeoPELMO DE.

It was further observed that runoff, macropore flow and drainage can lead to both reduced or increased estimated metabolite leachate concentrations in 1 m soil depth. It seems that increasing concentrations due to runoff were found when the parent compound was applied in autumn (e.g. winter cereals), and decreasing concentrations were found when the parent compound was applied in spring (e.g., maize). Considering macropore flow or drainage, it is rather difficult to describe the increase or decrease in percolate concentrations as a function of certain parameters or conditions. This is also due to the very low relative changes in metabolite percolate concentrations because of the implementation of these processes. A general explanation could be that the two processes runoff and macropore flow in PELMO are significantly influenced by the water balance in the uppermost soil layer and that drainage tends to take place close to 1 m soil depth. In contrast, the formation and transport of metabolites take place gradually in the soil column and is therefore less influenced by these processes.

The combined influence of all three additional processes on the nationwide metabolite percolate concentrations is finally provided in Table 71 and Table 72. The ratio of the leaching results from both modelling runs (FOCUS L and FOCUS L+R+M+D) provides evidence that slightly lower spatial median and spatial 80th percentile percolate concentrations are estimated for metabolites in spring applications if runoff, macropore flow and drainage are additionally considered in the modelling routine. The ratios of concentrations show a decreasing trend in a range between 0.90 and 0.98. In contrast, the ratio of the leaching results from both modelling runs (FOCUS L and FOCUS L+R+M+D) provides evidence that slightly higher spatial median and spatial 80th percentile percolate concentrations are estimated for metabolites in autumn applications if runoff, macropore flow and drainage are additionally considered in the modelling routine. The ratios of concentrations show an increasing trend in a range between 1.0 and 1.04. In one situation, the additional processes also lead to decreasing metabolite concentrations for autumn applications. Both slightly increasing and decreasing trends seem to be mainly driven by concentration changes due to runoff.

The spatial modelling results are sensitive to organic carbon contents in soil. It was shown that replacing the humus class h0 with slightly different default organic carbon contents leads to changes in metabolite leachate concentrations rather independent from individual crops, application timings and the spatial percentile selection. However, the effect is significantly lower for metabolites than for active substances.

Table 71: Combined influence of runoff, macropore flow and drainage on the spatial 80th percentile of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different active substances and two crops. The calculated ratio represents the decrease or increase of leachate concentrations due to the consideration of runoff, macropore flow and drainage. The results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

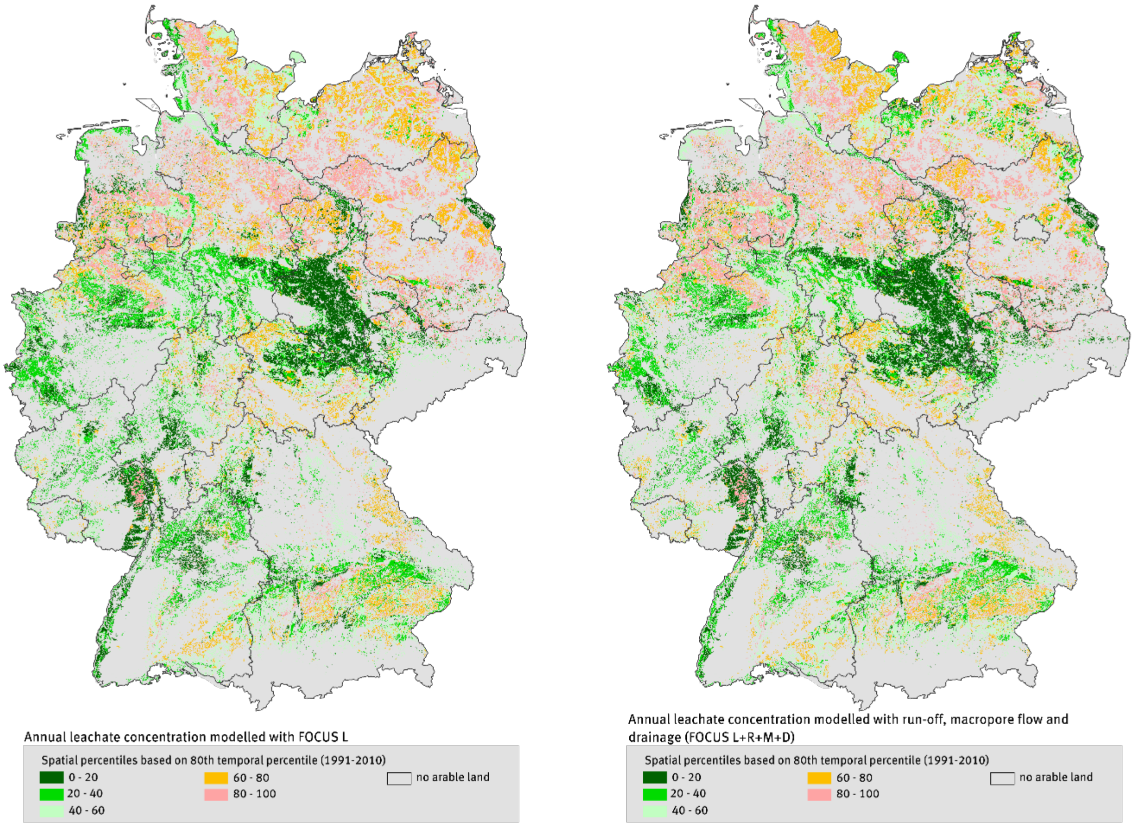
Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L [µg/L]	FOCUS L+R+M+D [µg/L]	Decreasing or increasing leachate concentrations (ratio) [-]
Maize	M2 (P1)	30	80	10.749	10.341	0.96
Maize	M1 (P2)	10	40	4.873	4.790	0.98
Maize	M2 (P2)	30	80	5.968	5.648	0.95
Maize	M2 (P3)	30	80	14.674	13.962	0.95
Winter cereals	M2 (P1)	30	80	19.954	20.112	1.01
Winter cereals	M1 (P2)	10	40	7.261	7.525	1.04
Winter cereals	M2 (P2)	30	80	8.794	8.784	1.00
Winter cereals	M2 (P3)	30	80	16.537	16.387	0.99

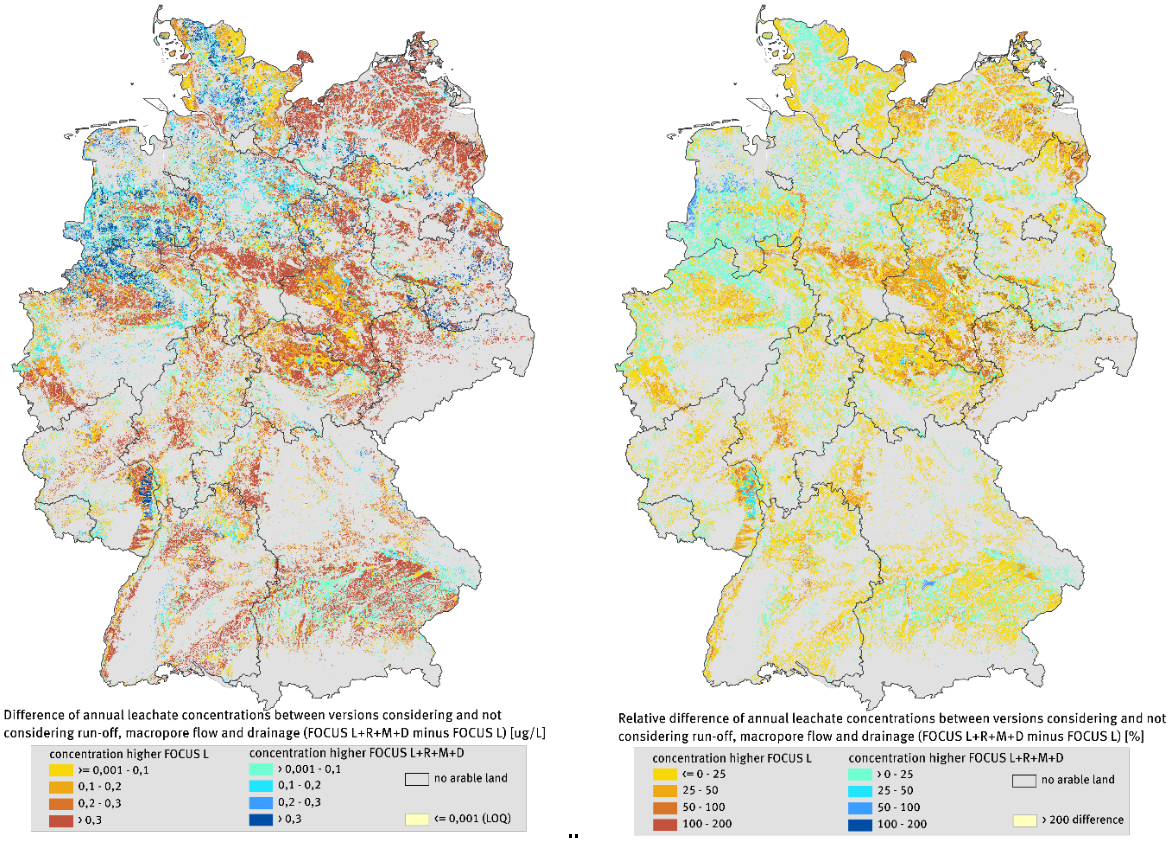
Table 72: Combined influence of runoff, macropore flow and drainage on the spatial median of annual leachate concentrations calculated with GeoPELMO DE

Model simulations are conducted for two dummy metabolites M1 and M2 formed from different dummy active substances and two crops. The calculated ratio represents the decrease or increase of leachate concentrations due to the consideration of runoff, macropore flow and drainage. The results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS L [µg/L]	FOCUS L+R+M+D [µg/L]	Decreasing or increasing leachate concentrations (ratio) [-]
Maize	M2 (P1)	30	80	8.245	7.645	0.93
Maize	M1 (P2)	10	40	3.561	3.190	0.90
Maize	M2 (P2)	30	80	4.373	4.104	0.94
Maize	M2 (P3)	30	80	10.405	9.971	0.96
Winter cereals	M2 (P1)	30	80	13.587	13.891	1.02
Winter cereals	M1 (P2)	10	40	5.212	5.133	0.98
Winter cereals	M2 (P2)	30	80	5.864	5.942	1.01
Winter cereals	M2 (P3)	30	80	11.103	11.138	1.00

Figure 79: Influence of runoff, macropore flow and drainage on leachate concentrations at 1 m soil depth calculated with GeoPELMO DE for dummy metabolite M1 formed from active substance P2 in maize





Source: own illustration, Fraunhofer IME.

The spatial influence of model results considering all three processes runoff, macropore flow and drainage in addition to chromatographic leaching is provided as an example in different maps in Figure 79 for dummy metabolite M1 formed from the active substance P2 after spring application in maize. In the map on the left, the spatially distributed annual leachate concentrations are shown as relative figure in five percentile classes based on the 80th temporal percentile according to 20 weather years from the FOCUS leaching concept (FOCUS L). The map on the right shows comparable concentrations based on modelling considering preferential flow, runoff and drainage (FOCUS L+R+M+D). The maps below show the absolute (left) and relative difference (right) in leachate concentrations depending on the different parameterisation of the model. The comparison analysis show that predicted metabolite leachate concentrations based on the FOCUS modelling routine are mainly higher in the northern belt in Germany with glacial deposits and sandy soils compared to the southern agricultural areas. The percentile classes or (relative concentrations) in the northern and southern areas do not change to a visual extent, if runoff, macropore flow and drainage are additionally considered in the modelling. In large agricultural areas, the estimated metabolite leachate concentrations decrease, while mainly north-western areas and some areas in Bavaria are characterised by increasing concentrations. However, the modelled concentrations for M1 are higher in total compared to the dummy active substances, which means that the relative difference of leachate concentrations for the metabolite M1 is rather small, if additional soil water processes are considered in the modelling with GeoPELMO DE. This was already shown in the tables above as general output for different dummy metabolite situations.

5.5 Analysis of the current level of protection

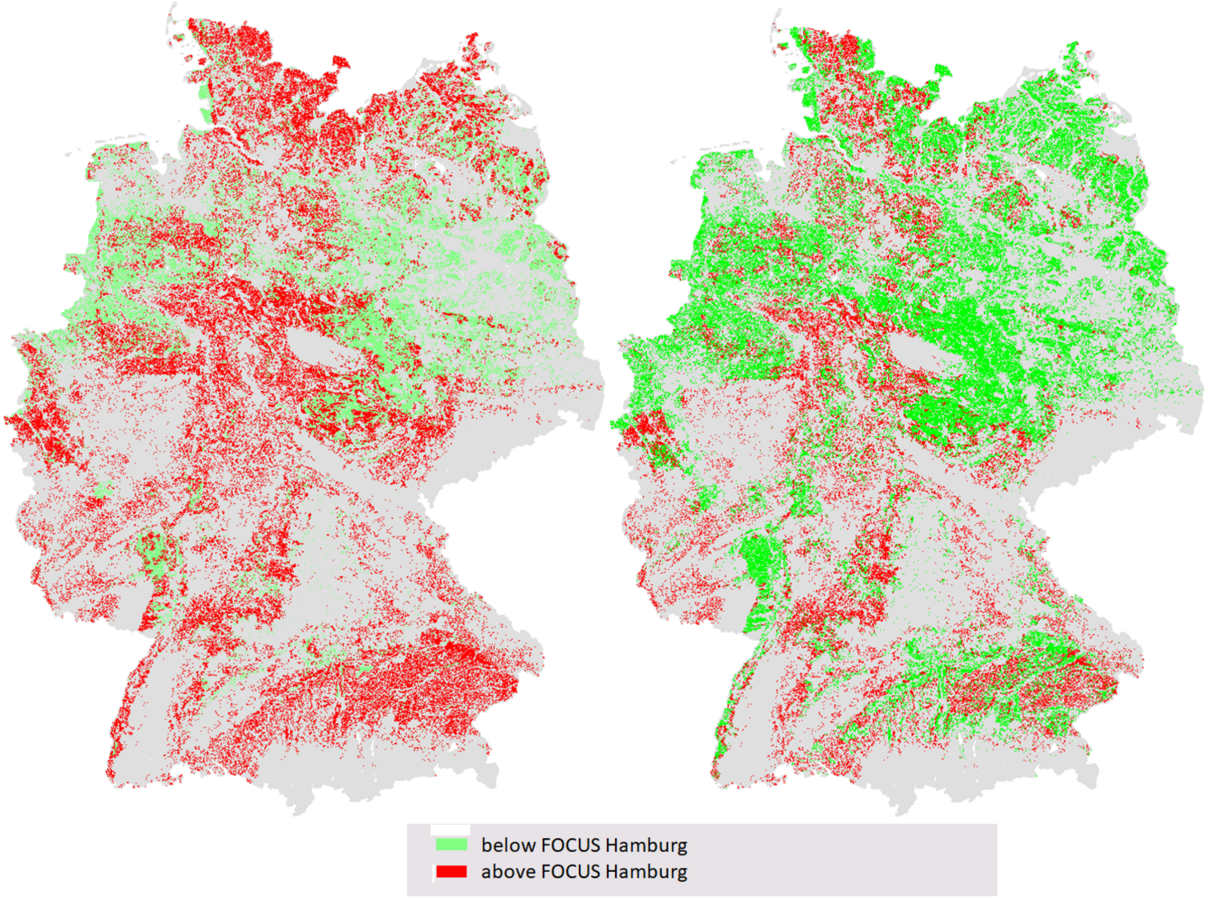
In the national regulatory framework for plant protection products, the FOCUS Hamburg scenario in combination with FOCUS PELMO is currently used as standard scenario to estimate leachate concentrations and the risk for groundwater. In this chapter an analysis is carried out to determine the level of protection for Germany covered by the FOCUS Hamburg scenario in comparison with GeoPELMO DE for active substances and metabolites. The evaluation of the protection level of the FOCUS Hamburg scenario is based on the analysis of the percentile, which the FOCUS Hamburg scenario represents within the nationwide agricultural area (arable land and permanent crops). The spatial percentile is calculated by comparing the predicted environmental (percolate) concentration (PEC) in FOCUS Hamburg with the predicted cumulative percolate concentrations of the entire agricultural area calculated with GeoPELMO DE. In addition, the combination of the 80th temporal and 80th spatial percentile (as realistic worst-case from spatial distributed leaching modelling), the combination of the 80th temporal and 90th spatial percentile and the combination of the 80th temporal and maximum spatial concentration are provided and compared with the PECs from the FOCUS Hamburg scenario.

5.5.1 Active substances

Nationwide average annual percolate concentrations are calculated and evaluated for three different fictive parent compounds (P1, P2, P3), whose properties differ in their sorption constants and their degradation rate in soil (see section 5.1). Results from different model versions are compared in the evaluation based on a sequence with five simulation runs with GeoPELMO DE (see section 5.2). Leachate concentrations in maize and winter cereals are estimated to represent two different pesticide application times in spring and autumn, respectively.

Figure 80: **Protection level of FOCUS Hamburg compared to nationwide simulations with GeoPELMO DE for dummy active substance P2 in different crops**

As an example, the predicted leachate concentration from the FOCUS Hamburg scenario is compared with nationwide leachate concentrations for the agricultural area in Germany. The simulation runs were conducted for maize (left) and winter cereals (right) with the model version inclusion runoff, macropore flow and drainage (FOCUS L+R+M+D). All PECs are based on the 80th temporal percentile of annual concentrations from 20 weather years (1991-2010). Green coloured areas are covered, and red coloured areas are not covered by the FOCUS Hamburg scenario.



Source: own illustration, Fraunhofer IME.

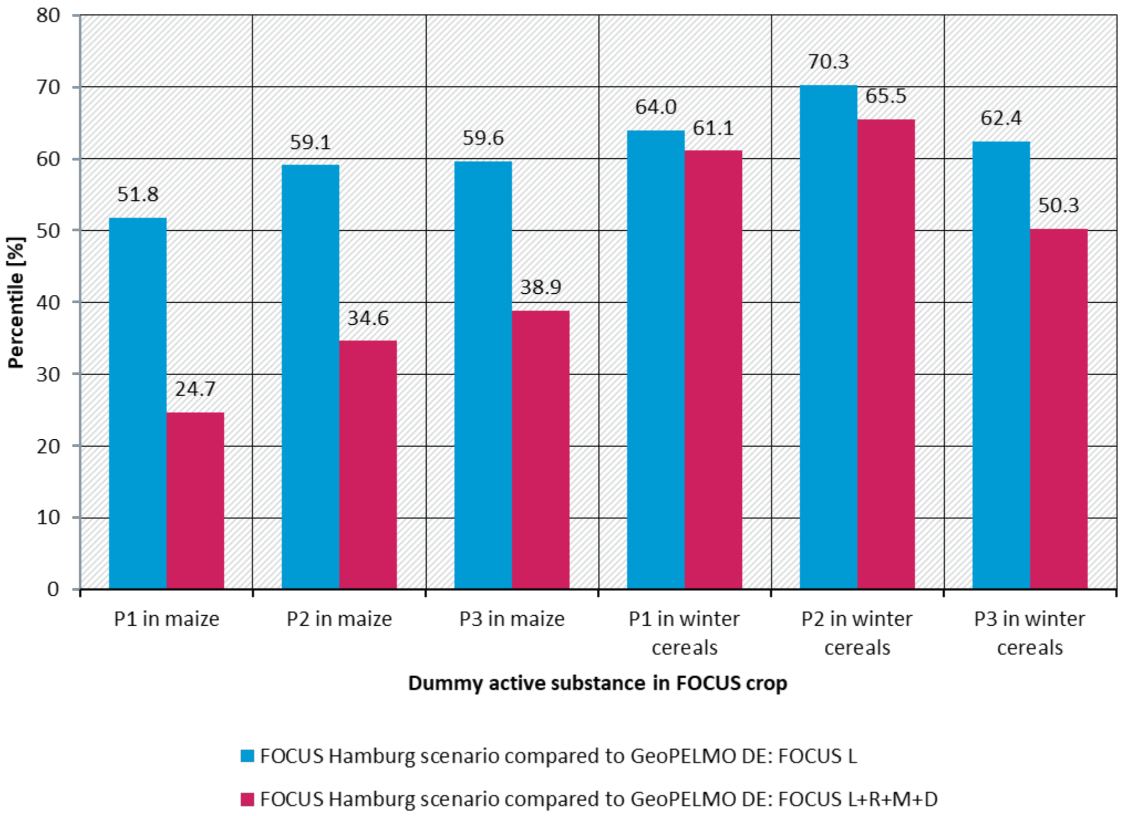
In Figure 80, an example is provided for the parent compound P2 (K_{foc}: 60 L/kg, $DegT_{50}$: 20 d) based on the model version of GeoPELMO DE including runoff, macropore flow and drainage as additional processes. The maps show areas that are protected for a spring application in maize and an autumn application in winter cereals when the predicted leachate concentration from the FOCUS Hamburg scenario is compared with nationwide leachate concentrations for the agricultural area in Germany. The green coloured areas represent soil-climate-conditions, which are covered by the FOCUS Hamburg scenario, whereas the red coloured areas stand for conditions, which are not covered, and their PECs are higher than the respective FOCUS Hamburg result. It could be expected that the PEC from the FOCUS Hamburg scenario represents a rather high percentile in the comparison with spatial distributed leaching modelling results. Covering around an 80th spatial percentile would fit into the concept that FOCUS Hamburg represents realistic worst-case climate-soil-conditions in Germany. However, especially in maize (Figure 80, left map) the red coloured areas are dominant. That means that according to the GeoPELMO DE results FOCUS Hamburg is not representing the 80th spatial percentile for German agricultural areas. Similar comparisons are also conducted for the dummy compounds P1 and

P3. The results of the protection level of the FOCUS Hamburg scenario are calculated and provided in Figure 81, Table 73 and Table 74 for all crops and all three active substances.

As an example, the predicted leachate concentration from the FOCUS Hamburg scenario is compared with nationwide leachate concentrations for the agricultural area in Germany. The simulation runs were conducted for maize (left) and winter cereals (right) with the model version inclusion runoff, macropore flow and drainage (FOCUS L+R+M+D). All PECs are based on the 80th temporal percentile of annual concentrations from 20 weather years (1991-2010). Green coloured areas are covered, and red coloured areas are not covered by the FOCUS Hamburg scenario.

Figure 81: Protection level of FOCUS Hamburg compared to GeoPELMO DE simulations for active substances

Model simulations are conducted for three dummy active substances P1, P2 and P3 and two crops according to chapter 5.1. The predicted environmental concentrations (PEC) from the FOCUS Hamburg scenario are compared with the 80th spatial percentile from GeoPELMO DE for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010). Results are presented for different model versions according to chapter 5.2.



Source: own illustration, Fraunhofer IME.

As shown in Figure 81, the annual percolate concentration from Hamburg (80th temporal percentile) for the three dummy active substances were found to be in the range of the 25th and the 66th percentile of nationwide distributed PECs when runoff, macropore flow and drainage are additionally considered in GeoPELMO DE. The arithmetic mean of the spatial percentiles was 46 %. This relative comparison indicate that the FOCUS Hamburg scenario is not representing the 80th spatial percentile for German climate and soil conditions, but rather a central spatial percentile is met by the FOCUS Hamburg scenario, only. The deviation from an expected 80th spatial percentile is higher for the spring applications in maize (25th-39th percentile) than for autumn applications in winter cereals (50th -66th percentile). The substance properties also show a strong influence on the percentile calculation. More information about the PECs is provided in Table 73. In Table 75, the ratios between the 80th percentile concentrations from GeoPELMO DE (FOCUS L+R+M+D) simulations and the FOCUS Hamburg scenario are additionally summarised for all dummy active substances and crops: The ratios are in the range of 1.9 to 11.0.

When only the FOCUS leaching concept of chromatographic flow is considered in GeoPELMO DE , and runoff, macropore flow and drainage are not included, the calculated percentiles for the FOCUS Hamburg scenarios are higher and in a range between 52 % and 70 % (Figure 81, Table 74). The average percentile for the three substances and both crops was found to be 61 %. This is in line with previous results. It was proven that runoff, macropore flow and drainage lead overall to increased leachate concentrations for active substances. This must lead to lower percentiles of the FOCUS Hamburg results. Conversely, the exclusion of these processes leads to a higher level of protection for FOCUS Hamburg. Nevertheless, it can be observed that the FOCUS Hamburg scenario is still not representing the 80th spatial percentile for German climate and soil conditions if the FOCUS leaching concept is transferred to nationwide conditions. The deviation from an expected 80th spatial percentile is still higher for the spring applications in maize (62nd-60th percentile) than for autumn applications in winter cereals (62nd- 70th percentile). In Table 75 the ratios between the 80th percentile concentrations from GeoPELMO DE simulations (FOCUS L) and the FOCUS Hamburg scenario are summarised: The ratios are in a range between 1.7 and 4.4. Considering the PELMO version with runoff, macropore flow and drainage the ratios are quite comparable for all simulations in winter cereals, whereby the ratios are lower for simulations in maize.

Table 73: Comparison of results from FOCUS PELMO Hamburg scenario with GeoPELMO DE including runoff, drainage and macropore flow with a dynamic fraction of 4-8 %

Model simulations are conducted for three dummy active substances and two crops. All provided values are based on the 80th temporal percentiles from 20 weather years (1991-2010). The spatial percentile of FOCUS Hamburg scenario represents the percentage of the agricultural area in Germany, which is covered by the PEC Hamburg.

Crop	Active sub-stance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS Hamburg spatial perc. [%]	FOCUS Hamburg [µg/L]	GeoPELMO DE FOCUS L+R+M +D 80th p. [µg/L]	GeoPELMO DE FOCUS L+R+M +D 90th p. [µg/L]	GeoPELMO DE FOCUS L+R+M +D 100th p. [µg/L]
Maize	P1	30	10	24.7	0.005	0.055	0.092	1.352
Maize	P2	60	20	34.6	0.029	0.145	0.208	1.767
Maize	P3	240	80	38.9	0.057	0.257	0.415	4.227
Winter cereals	P1	30	10	61.1	0.400	0.896	1.726	15.364
Winter cereals	P2	60	20	65.5	0.328	0.626	1.071	12.313
Winter cereals	P3	240	80	50.3	0.137	0.414	0.705	7.067

Table 74: Comparison of results from FOCUS PELMO Hamburg scenario with GeoPELMO DE based on the FOCUS version without runoff, macropore flow and drainage

Model simulations are conducted for three dummy active substances and two crops. All provided values are based on the 80th temporal percentiles from 20 weather years (1991-2010). The spatial percentile of FOCUS Hamburg scenario represents the percentage of the agricultural area in Germany, which is covered by the PEC Hamburg.

Crop	Active sub-stance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS Hamburg spatial perc. [%]	FOCUS Hamburg [µg/L]	GeoPELMO DE FOCUS L+R+M +D 80th p. [µg/L]	GeoPELMO DE FOCUS L+R+M +D 90th p. [µg/L]	GeoPELMO DE FOCUS L+R+M +D 100th p. [µg/L]
Maize	P1	30	10	51.8	0.005	0.022	0.040	1.565
Maize	P2	60	20	59.1	0.029	0.088	0.192	1.936
Maize	P3	240	80	59.6	0.057	0.205	0.458	4.554
Winter cereals	P1	30	10	64.0	0.400	0.930	1.828	15.120
Winter cereals	P2	60	20	70.3	0.328	0.568	1.117	12.142
Winter cereals	P3	240	80	62.4	0.137	0.379	0.773	7.974

Table 75: Comparison of results from FOCUS PELMO Hamburg scenario with GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops. All provided values are based on the 80th temporal percentiles from 20 weather years (1991-2010). The spatial percentile of FOCUS Hamburg scenario represents the percentage of the agricultural area in Germany, which is covered by the PEC Hamburg. The ratio is calculated as quotient between the PEC representing the 80th spatial percentile from GeoPELMO DE and the PEC from the FOCUS Hamburg scenario.

Crop	Active sub-stance	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS Hamburg [µg/L]	Ratio: 80th p. GeoPELMO DE (FOCUS L+R+M+D) / FOCUS Hamburg [-]	Ratio: 80th p. GeoPELMO DE (FOCUS L) / FOCUS Hamburg [-]
Maize	P1	30	10	0.005	11.0	4.4
Maize	P2	60	20	0.029	5.0	3.0
Maize	P3	240	80	0.057	4.5	3.6
Winter cereals	P1	30	10	0.400	2.2	2.3
Winter cereals	P2	60	20	0.328	1.9	1.7
Winter cereals	P3	240	80	0.137	3.0	2.8

The results presented so far were all referring to the GeoPELMO DE model version based on the FOCUS leaching approach (FOCUS L: chromatographic flow only) and a version including three additional processes (FOCUS L+R+M+D: + runoff, macropore flow and drainage). In the following, the spatial percentile analysis is performed for a sequence of several simulation runs according to different model parametrisations provided in chapter 5.2. In the simulation sequence additional processes are switched on, partly with different parametrisations. This analysis illustrates the contribution of the individual processes and different parametrisations to the discrepancy that the FOCUS Hamburg scenario does not reach a rather high spatial percentile in comparison with nationwide modelling results with GeoPELMO DE (see Table 76). The results demonstrate that the model variations have a significant influence on the calculated percentile for the FOCUS Hamburg scenario.

Table 76: Spatial percentile of the FOCUS PELMO Hamburg scenario compared with results from different model versions of GeoPELMO DE

Model simulations are conducted for three dummy active substances and two crops. All provided values are based on the 80th temporal percentiles from 20 weather years (1991-2010). Different model parametrisations of GeoPELMO DE are considered according to chapter 5.2. The spatial percentile of FOCUS Hamburg scenario represents the percentage of the agricultural area in Germany, which is covered by the PEC Hamburg.

		Percentile FOCUS PELMO Hamburg scenario compared to GeoPELMO DE						
Crop	**Active sub-stance**	**FOCUS L**	**FOCUS L+R**	**FOCUS L+R+M (4-8 %) standard:**	**FOCUS L+R+M (2-5 %)**	**FOCUS L+R+M (5-10 %)**	**FOCUS L+R+M+D**	**FOCUS L+R+M+D (OC: 0.2 %)**
Maize	P1	**51.8**	68.3	20.8	23.2	20.4	**24.7**	28.8
Maize	P2	**59.1**	72.2	31.1	35.7	29.8	**34.6**	40.6
Maize	P3	**59.6**	70.7	36.6	41.8	34.8	**38.9**	48.3
Winter cereals	P1	**64.0**	65.1	58.0	62.7	54.0	**61.1**	67.4
Winter cereals	P2	**70.3**	71.5	63.8	68.4	60.4	**65.5**	72.3
Winter cereals	P3	**62.4**	66.5	49.2	59.8	42.2	**50.3**	65.6

If runoff is included in the GeoPELMO DE simulation (FOCUS L+R) the calculated percentiles for the FOCUS Hamburg scenario referring to P1-P3 in two different crops increase and get closer to the 80th percentile (range 65 % to 72 %). The increase compared to GeoPELMO DE based on the FOCUS approach (FOCUS L) is rather large with 11-16 % for spring application in maize, but rather low with 1-4 % for autumn application in winter cereals. The increase itself is not surprising since runoff reduces the percolate concentrations to a certain extent. The consequence is that a lower range of nationwide concentrations is calculated with GeoPELMO DE and the FOCUS Hamburg is representing a higher percentile.

The situation is different if macropore flow with the standard dynamic parametrisation of 4-8 % is added in GeoPELMO DE (FOCUS L+R+M). The calculated concentrations are significantly increasing at a large proportion agricultural area. Consequently, FOCUS Hamburg represents lower spatial percentiles in a range between 21 % and 64 %. Furthermore, the results show that macropore flow is predominantly affecting the percentiles for applications in spring (maize). The reduce of the percentile compared to GeoPELMO DE with runoff (FOCUS L+R) is significant with 34-48 % for spring application in maize, and with 7-17 % lower for autumn application in winter cereals.

The protection level of FOCUS Hamburg is also provided for a dynamic macropore flow parametrisation of 2-5 % and 5-10 %. The parametrisation of 2-5 % leads to slightly higher percentiles in a range between 23 % and 68 %. The increase compared to the standard macropore flow (4-8 %) is about 2-5 %. The parametrisation of 5-10 % leads to slightly lower percentiles in a range between 20 % and 60 %. The reduce in the simulations compared to the standard macropore flow (4-8 %) is about 0-7 %. It leads to the conclusion that including macropore flow in GeoPELMO DE has a larger effect on the protection level of FOCUS Hamburg than different tested macropore flow parametrisations.

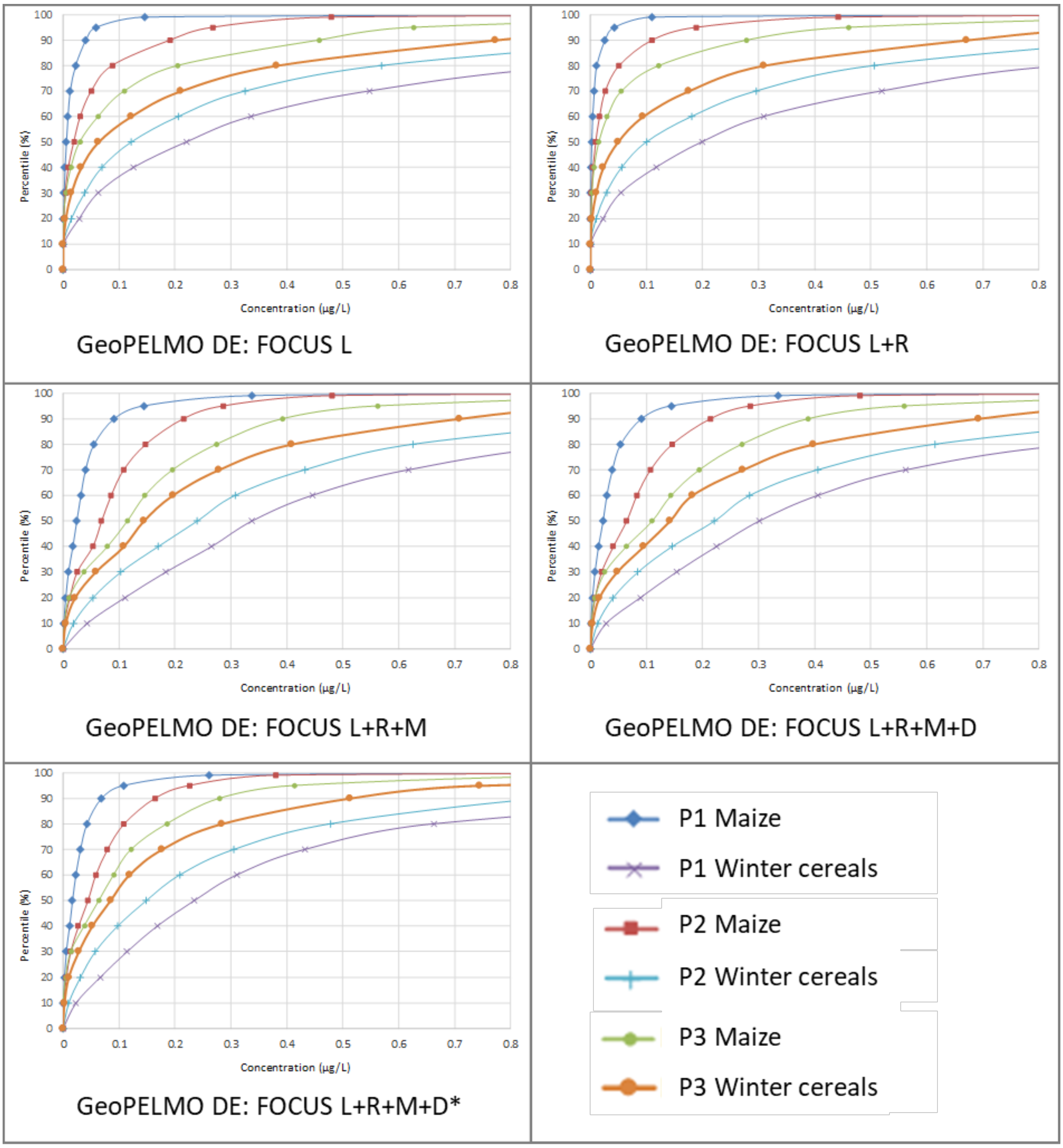
Including drainage in GeoPELMO DE (FOCUS L+R+M+D) has a minor effect on the percentile calculations for the FOCUS Hamburg scenario. This is in line with previous findings that drainage has a rather small effect on the estimated percolate concentrations for active substances at 1 m soil depth. Considering drainage, FOCUS Hamburg represents higher spatial percentiles in a range between 25 % and 66 %. The increase of percentiles compared to GeoPELMO DE (FOCUS L+R+M) with the standard macropore flow (4-8 %) is about 1-4 %.

In a last simulation, the influence of a default organic carbon content of 0.2 % for humus class 0 in subsoils (instead of 0.1 % and 0.2 % for different soil depths) was evaluated for the protection level of the FOCUS Hamburg scenario compared to nationwide estimations with GeoPELMO DE (FOCUS L+R+M+D). A slightly higher default value of the organic carbon content leads to lower nationwide percolate concentrations and higher percentiles of FOCUS Hamburg scenario in the range of 29 % to 72 %. The increase of the percentiles between 4 % and 15 % is observed to be rather independent of the application time and crops but influenced by the properties of the active substances.

Table 76 showed the influence of the different processes and parametrisations in GeoPELMO DE on the level of protection for the FOCUS Hamburg scenario calculated by percentiles. In the following, the effect of different model parametrisations (see Figure 82), and the influence of active substance properties and application times (see Figure 83) on nationwide modelling results are presented by cumulative distribution curves. The curves in Figure 82 show how the relative conservativeness of the different model variations changes with a given percentile. As evaluated before, GeoPELMO DE versions including runoff (FOCUS L+R) and with a higher default organic carbon content for humus class h0 are less conservative than other model versions. In the diagrams it can be observed that they reach high percentiles already at low concentrations. The curves in Figure 83 show that the steepness of the curves depends also on substance properties and application times. Sometimes the cumulative curves cross each other, which means that the relative conservativeness of a model version changes at different percentiles.

Figure 82: Cumulative distribution curves for GeoPELMO DE simulations with different processes and parametrisations

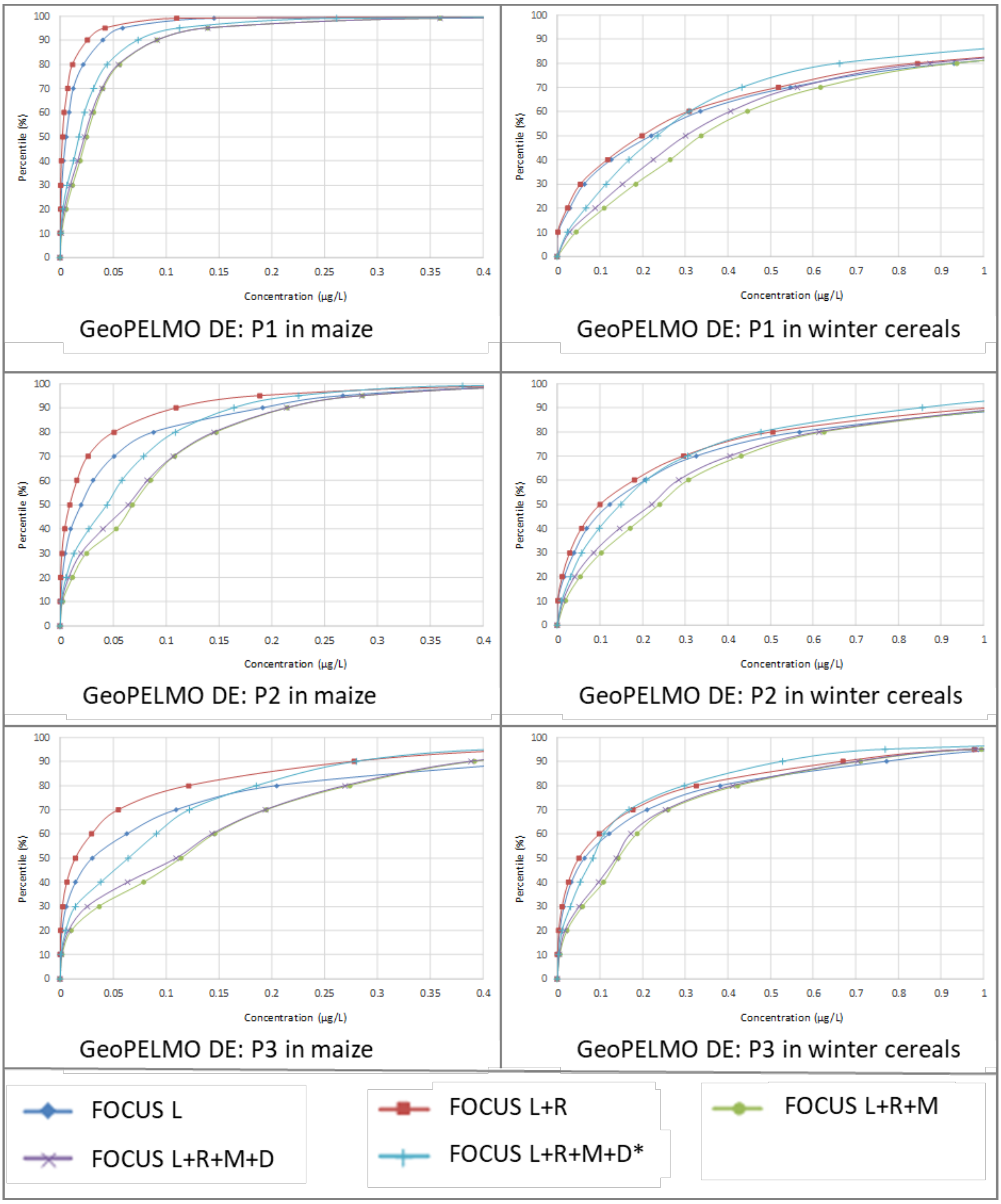
Model simulations are conducted for three dummy active substances P1, P2 and P3 and two crops according to chapter 5.1. The predicted environmental concentration (PEC) from the FOCUS Hamburg scenario is compared with the 80th spatial percentile from GeoPELMO DE for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010). Results are presented for different model versions according to chapter 5.2.



* GeoPELMO DE simulation was conducted with 0.2 % default organic carbon content for humus class h0.
Source: own illustration, Fraunhofer IME.

Figure 83: Cumulative distribution curves for GeoPELMO DE simulations with different active substances and application times

Model simulations are conducted for different model versions according to chapter 5.2. Cumulative distribution curves for the agricultural area in Germany are based on the 80th temporal percentiles from 20 weather years (1991-2010). Results are presents for three dummy active substances P1, P2 and P3 and two crops according to chapter 5.1.



* GeoPELMO DE simulation was conducted with 0.2 % default organic carbon content for humus class h0.

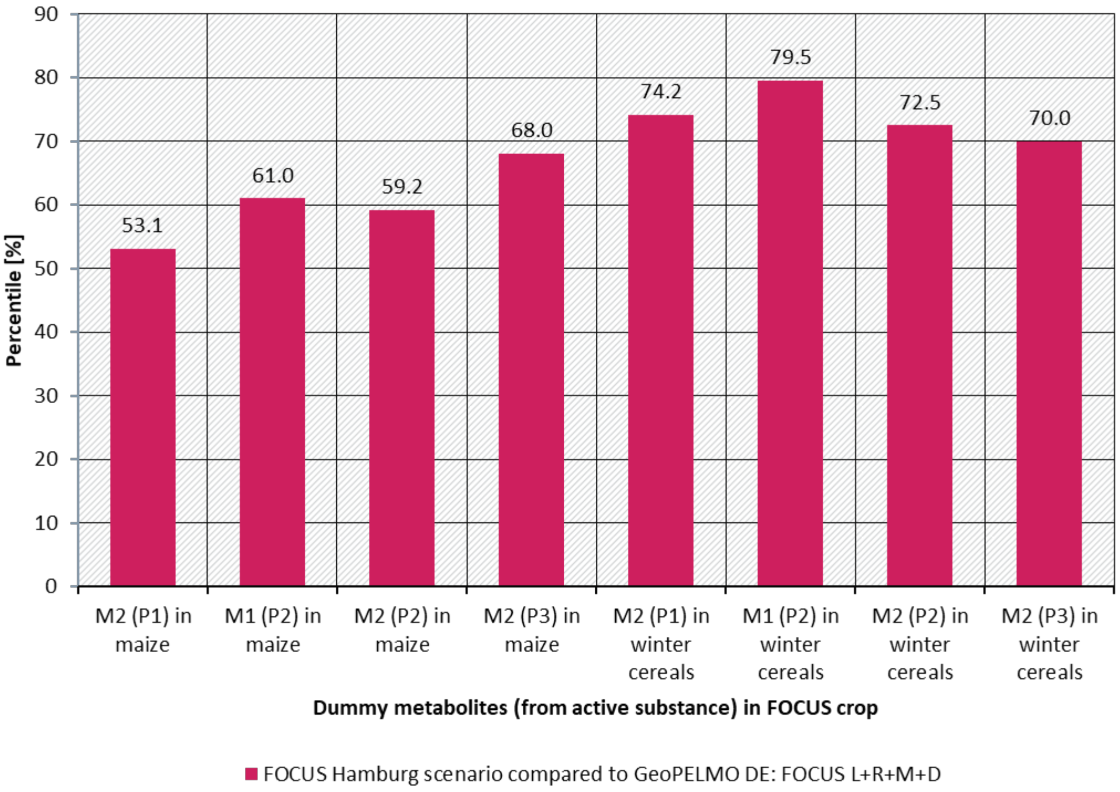
Source: own illustration, Fraunhofer IME.

5.5.2 Metabolites

In this chapter an evaluation is performed for two dummy transformation products formed from different fictive active substances. As already shown in chapter 5.4.2, the influence of additional processes like runoff, macropore flow and drainage on spatial distributed percolate concentrations calculated with GeoPELMO DE is very limited for these transformation products. Therefore, only results for one simulation run with GeoPELMO DE (FOCUS L+R+M+D) including all additional processes are presented in Figure 84 and Table 77. The calculated percentiles of the FOCUS Hamburg scenario compared to nationwide leachate concentrations were found to be in the range of 53 % (M2 formed by P1 in maize) and 80 % (M1 formed by P2 in winter cereals). The average percentile over both crops and all fictive transformation products was found to be 67 %. The percentiles seem to be higher for the autumn applications in winter cereals (range between 70 % and 80 %) compared to spring applications in maize (range between 53 % and 68 %). Compared to the evaluations for active substances higher spatial percentiles are reached with the FOCUS Hamburg scenarios for the two dummy metabolites. However, it has to be admitted that the evaluated number of metabolites is rather small for that conclusion.

Figure 84: Protection level of FOCUS Hamburg compared to GeoPELMO DE simulations for metabolites

Model simulations are conducted for two dummy metabolites M1 and M2 formed from three dummy active substances P1, P2 and P3 and two crops according to chapter 5.1. The predicted environmental concentration (PEC) from the FOCUS Hamburg scenario is compared with the 80th spatial percentile from GeoPELMO DE for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010). Results are presented for one model versions according to chapter 5.2.



Source: own illustration, Fraunhofer IME.

Table 77 provides some more details about the respective percolate concentrations calculated for the FOCUS Hamburg scenario and estimated with GeoPELMO DE (FOCUS L+R+M+D). It demonstrates that the concentrations of FOCUS Hamburg are rather close and comparable to the 80th and 90th spatial percentile calculated with GeoPELMO DE. However, the maximum concentration of GeoPELMO DE was found to be significantly higher. That means that this situation represents rather extreme than realistic worst-case conditions.

Table 77: Comparison of results from FOCUS PELMO Hamburg scenario with GeoPELMO DE including runoff, macropore flow with a dynamic fraction of 4-8 % and drainage

Model simulations are conducted for two dummy metabolites from different active substances and two crops. All provided values are based on the 80th temporal percentiles from 20 weather years (1991-2010). The spatial percentile of FOCUS Hamburg scenario represents the percentage of the agricultural area in Germany, which is covered by the PEC Hamburg.

Crop	Meta-bolite	FOCUS Hamburg spatial percent. [%]	FOCUS Hamburg [µg/L]	GeoPELMO DE FOCUS L+R+M+D 80th percentile [µg/L]	GeoPELMO DE FOCUS L+R+M+D 90th percentile [µg/L]	GeoPELMO DE FOCUS L+R+M+D 100th percentile [µg/L]
Maize	M2 (P1)	53.1	7.885	10.341	11.680	60.053
Maize	M1 (P2)	61.0	3.583	4.790	5.736	19.703
Maize	M2 (P2)	59.2	4.506	5.648	6.504	29.952
Maize	M2 (P3)	68.0	11.944	13.955	16.190	70.504
Winter cereals	M2 (P1)	74.2	18.287	20.109	23.420	121.970
Winter cereals	M1 (P2)	79.5	7.486	7.520	9.425	38.798
Winter cereals	M2 (P2)	72.5	7.650	8.784	9.974	50.650
Winter cereals	M2 (P3)	70.0	13.808	16.387	18.484	98.008

6 Recommendations for the national groundwater risk assessment

6.1 Derivation of national scenarios

Considering the results of the analysis of the spatial protection level of the FOCUS Hamburg scenario in chapter 5.5, a further analysis was conducted to derive alternative leaching scenarios for Germany. In section 6.1.2, the scenario selection is based on modelling results from the GeoPELMO DE (version FOCUS L) considering FOCUS leaching approach with chromatographic flow. In section 6.1.3, the GeoPELMO DE (version FOCUS L+R+M+D) considering chromatographic and preferential flow, runoff and drainage is used to select adequate scenarios.

6.1.1 Methodology

Regions and locations are identified for scenario selection which represent around the 80th spatial percentile of the nationwide agricultural area according to estimated nationwide percolate concentrations with GeoPELMO DE. A range between the 75th and the 85th percentile (80 ± 5 %) was considered to receive a reasonable area for the selection of relevant scenarios (see example maps for active substances in Figure 86 and for metabolites in Figure 87). The analysis is based on modelling results for three dummy active substances P1, P2, P3, two dummy metabolites M1 and M2 formed from different active substances and applications one day before emergence in maize and winter cereals (see chapter 5.1). This leads to nationwide percolate concentration maps for 14 different compound-crop situations which are used as basis for scenario selection. Before looking at the spatial distributed results (80 ± 5 % percentiles), the 80th temporal percentile of the predicted leachate concentrations in 1 m soil depth from a 20 years simulation period (1991-2010) was preselected.

The following principles are applied to identify two alternative realistic worst-case leaching scenarios based on GeoPELMO DE (FOCUS L) representing the FOCUS leaching modelling approach (see Figure 85):

- In **step A**, scenarios were selected based on the highest possible number of overlaps of all 14 percolate concentration maps in the range between the 75th and 85th spatial percentile.

The following principles are applied to identify alternative realistic worst-case leaching scenarios based on GeoPELMO DE (FOCUS L+R+M+D) considering chromatographic and preferential flow, runoff and drainage (see Figure 85):

- In **step B**, scenarios were selected based on the highest number of overlaps of all 14 percolate concentration maps in the range between the 75th and 85th spatial percentile.
- In **step C**, scenarios were selected based on 6 overlaps of all percolate concentration maps for active substances in the range between the 75th and 85th spatial percentile.
- In **step D**, scenarios were selected based on 8 overlaps of all percolate concentration maps for metabolites in the range between the 75th and 85th spatial percentile.
- In **step E**, scenarios were selected based on overlaps of all three percolate concentration maps for active substances P1-P3 in maize in the range between the 75th and 85th spatial percentile.

- In **step F**, scenarios were selected based on overlaps of all three percolate concentration maps for active substances P1-P3 in winter cereals in the range between the 75th and 85th spatial percentile.
- In **step G**, scenarios were selected based on overlaps of two percolate concentration maps for active substances P1 (with high mobility) in maize and winter cereals in the range between the 75th and 85th spatial percentile.
- In **step H**, scenarios were selected based on overlaps of two percolate concentration maps for active substances P2 (with moderate mobility) in maize and winter cereals in the range between the 75th and 85th spatial percentile.
- In **step I**, scenarios were selected based on overlaps of two percolate concentration maps for active substances P3 (with lower mobility) in maize and winter cereals in the range between the 75th and 85th spatial percentile.
- In **step K**, scenarios were selected based on overlaps of four percolate concentration maps for all metabolite situations in maize in the range between the 75th and 85th spatial percentile.
- In **step L**, scenarios were selected based on overlaps of four percolate concentration maps for all metabolite situations in winter cereals in the range between the 75th and 85th spatial percentile.

Figure 85: Concept to derive national scenarios based on GeoPELMO DE simulations

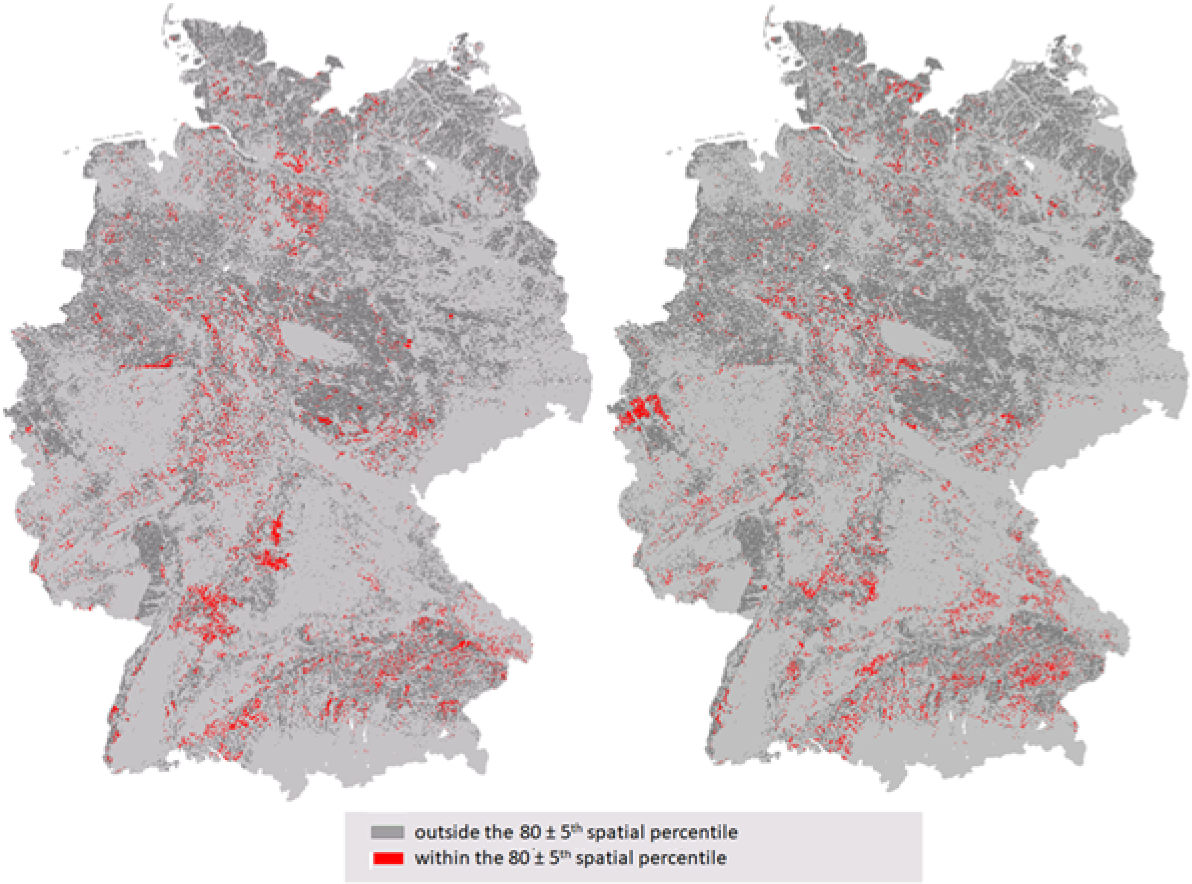
Fourteen model simulation runs are conducted for three dummy active substances P1, P2 and P3, two dummy metabolites M1 and M2 in maize and winter cereals according to chapter 5.1. The concept of scenario selection is based on the overlap of the 75th-85th spatial percentile from different simulation runs. Nationwide PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Spatial percentile		75-85	75-85	75-85	75-85	75-85	75-85	75-85	75-85	75-85	75-85	75-85	75-85	75-85	75-85
Application in…		maize	maize	maize	maize	maize	maize	maize	winter cereal	winter cereal	winter cereal	winter cereal	winter cereal	winter cereal	winter cereal
Dummy compound		P1	P2	P3	M2 (P1)	M1 (P2)	M2 (P2)	M2 (P3)	P1	P2	P3	M2 (P1)	M1 (P2)	M2 (P2)	M2 (P3)
Model version		**GeoPELMO DE (FOCUS L): FOCUS leaching concept: chromatigraphic flow**													
Step A	most possible overlaps of all simulation runs	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨
Model version		**GeoPELMO DE (FOCUS L+R+M+D): chromatigraphic flow + runoff, macropore flow, drainage**													
Step B	most possible overlaps of all simulation runs	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨
Step C	most possible overlaps for all active substances	▨	▨	▨					▨	▨	▨				
Step D	most possible overlaps for all metabolites				▨	▨	▨	▨				▨	▨	▨	▨
Step E	overlaps for all active substances in maize	▨	▨	▨											
Step F	overlaps for all active sub-stances in winter cereals								▨	▨	▨				
Step G	overlaps for very mobil active substance	▨							▨						
Step H	overlaps for moderate mobil active substance		▨							▨					
Step I	overlaps for less mobil active substance			▨							▨				
Step K	overlaps for all metabolites in maize				▨	▨	▨	▨							
Step L	overlaps for all metabolites in winter cereals											▨	▨	▨	▨

Source: own illustration, Fraunhofer IME.

Figure 86: Distribution of the 80 ± 5th spatial percentiles of annual leachate concentrations at 1 m soil depth for dummy active substance P2 in maize (left) and winter cereals (right)

Model simulations are conducted with the GeoPELMO DE version (FOCUS L+R+M+D) including runoff, macropore flow and drainage. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

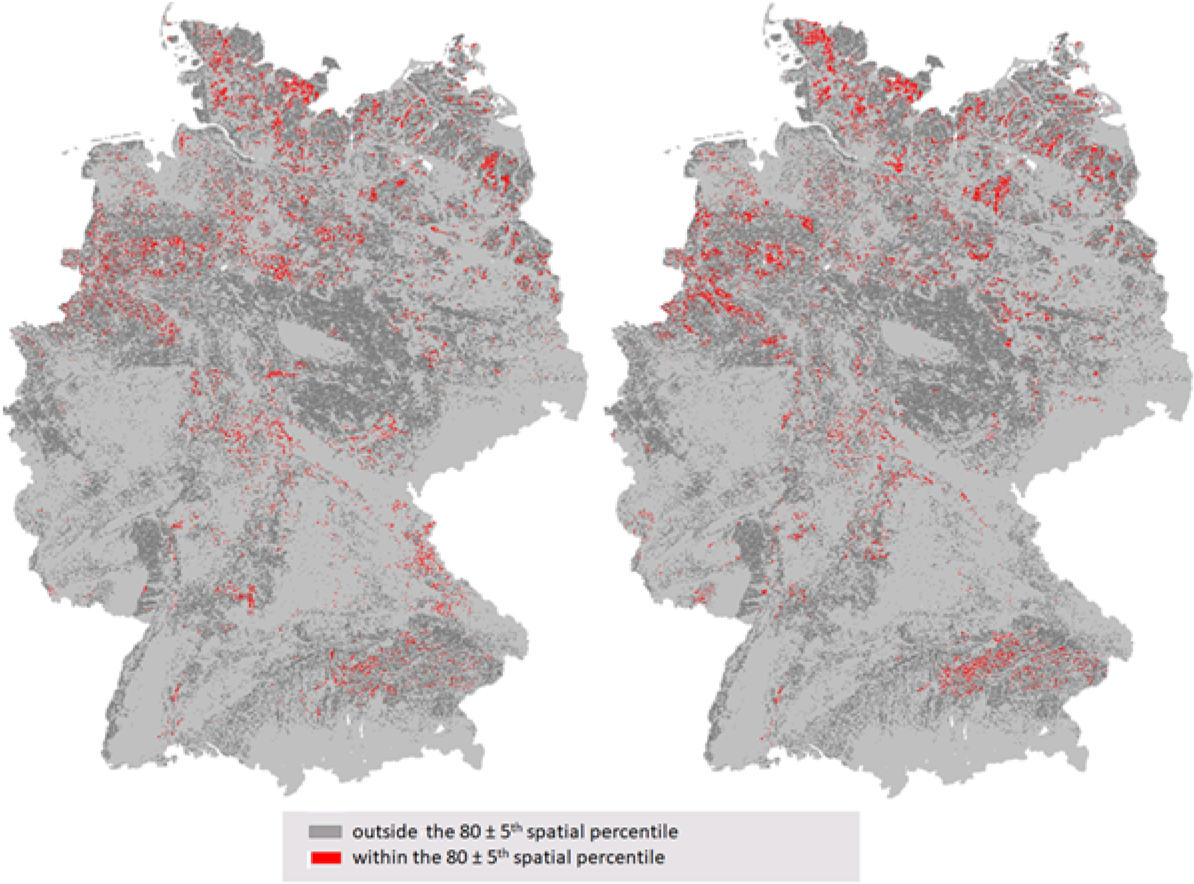


Source: own illustration, Fraunhofer IME.

There is some overlap between the two maps in Figure 86, but there are also regions where only one of the crops has its individual 80th spatial percentile. This result can be expected since applications in autumn (here: winter cereals) usually lead to different leaching behaviour compared to spring applications (here: maize) and consequently also to different nationwide vulnerability pattern. The results for another example are shown in Figure 87. Metabolite M1 is formed from active substance P2. Compared to the previous figure (active substance P2), there are larger areas in the north of Schleswig-Holstein marked as 80th percentile in both maps. However, there is also some overlap between the four maps (e.g. in Bavaria). Similar leaching maps are provided for all 14 crop-compound-combinations in appendix B.

Figure 87: Distribution of the 80 ± 5th spatial percentiles of annual leachate concentrations at 1 m soil depth for dummy metabolite M1 formed from active substance P2 in maize (left) and winter cereals (right)

Model simulations are conducted with the GeoPELMO DE version (FOCUS L+R+M+D) including runoff, macropore flow and drainage. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

6.1.2 Scenarios based on the FOCUS modelling approach considering chromatographic flow

According to current EU guidance (e.g., European Commission 2014) macropore flow, drainage and runoff are not considered to estimate the leaching risk of pesticides for groundwater via modelling. Referring to the methodology described in **step A** above, two realistic worst-case scenarios were identified when only chromatographic flow is considered in simulations with GeoPELMO DE (FOCUS L). Because there is no area with an overlap of all 14 concentration maps between the 75th and 85th spatial percentile, both climate-soil-scenarios represent the highest possible number of overlaps. The climate-soil combination with number 6739, soil profile number 2804 and weather station 'Barsinghausen-Hohenbostel' (ID: 6739/2804/Barsinghausen-Hohenbostel) was identified to represent an overlap for all 6 concentration maps for the active substances and the highest possible number of 7 overlaps of all 8 metabolite maps. The climate-soil combinations with number 6126, soil profile number 2620 and weather station 'Hohwacht' (ID: 6126/2620/Hohwacht) was selected and represents an optimal overlap for all 8 concentration maps for the metabolites and the highest possible number of 3 overlaps of 6 active substance maps. An overview of typical properties of both scenarios is presented in Table 78. Table 79 and Table 80 provide depth dependent soil properties as parameterised in GeoPELMO DE.

Table 78: Properties of climate-soil combinations from selection step A

Combination No.	**6739**	**6126 (6135^)**
Soil number	2804	2620
Climate Station	Barsinghausen-Hohenbostel	Hohwacht
Average annual precipitation (mm)	733	698
Average annual air temperature (°C)	9.9	9.3
Soil description (in German)	Pseudogley-Braunerden aus (sandiger) Lehmfließerde über Terrassenkies oder Hochflutlehm	Parabraunerden mit Pseudogleyen aus Geschiebelehm über (tiefem) Geschiebemergel vergesellschaftet mit Pararendzinen aus Geschiebemergel
Organic carbon content, top soil/0-1 m (%)	0.87/0.36	0.87/0.37
Average clay/silt/sand content (%)	10/22/68	17/35/48
Macropore flow	not considered°	not considered°
Drainage	not considered	not considered
Runoff	not considered	not considered
Selection step	A	A
Number of overlaps for active substances (maximum 6)	6	3
Number of overlaps for metabolites (maximum 8)	7	8
Agricultural area (km²)	2	24

^ Combination number 6126 changes to number 6135 if drainage is included in GeoPELMO DE (FOCUS L+R+M+D)

° The same soil profile in the GeoPELMO DE (FOCUS L+R+M+D) contains macropore class 2.

Table 79: Detailed information for soil profile 2804 (used in combination 6739)

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	30	1.99	0.24	0.09	0.87	1.0
2	15	2.05	0.22	0.09	0.2	0.5
3	5	1.99	0.24	0.11	0.2	0.5
4	15	1.99	0.24	0.11	0.2	0.3
5	35	2.15	0.18	0.06	0.1	0.3

Table 80: Detailed information for soil profile 2620 (used in combination 6135 and 6126)

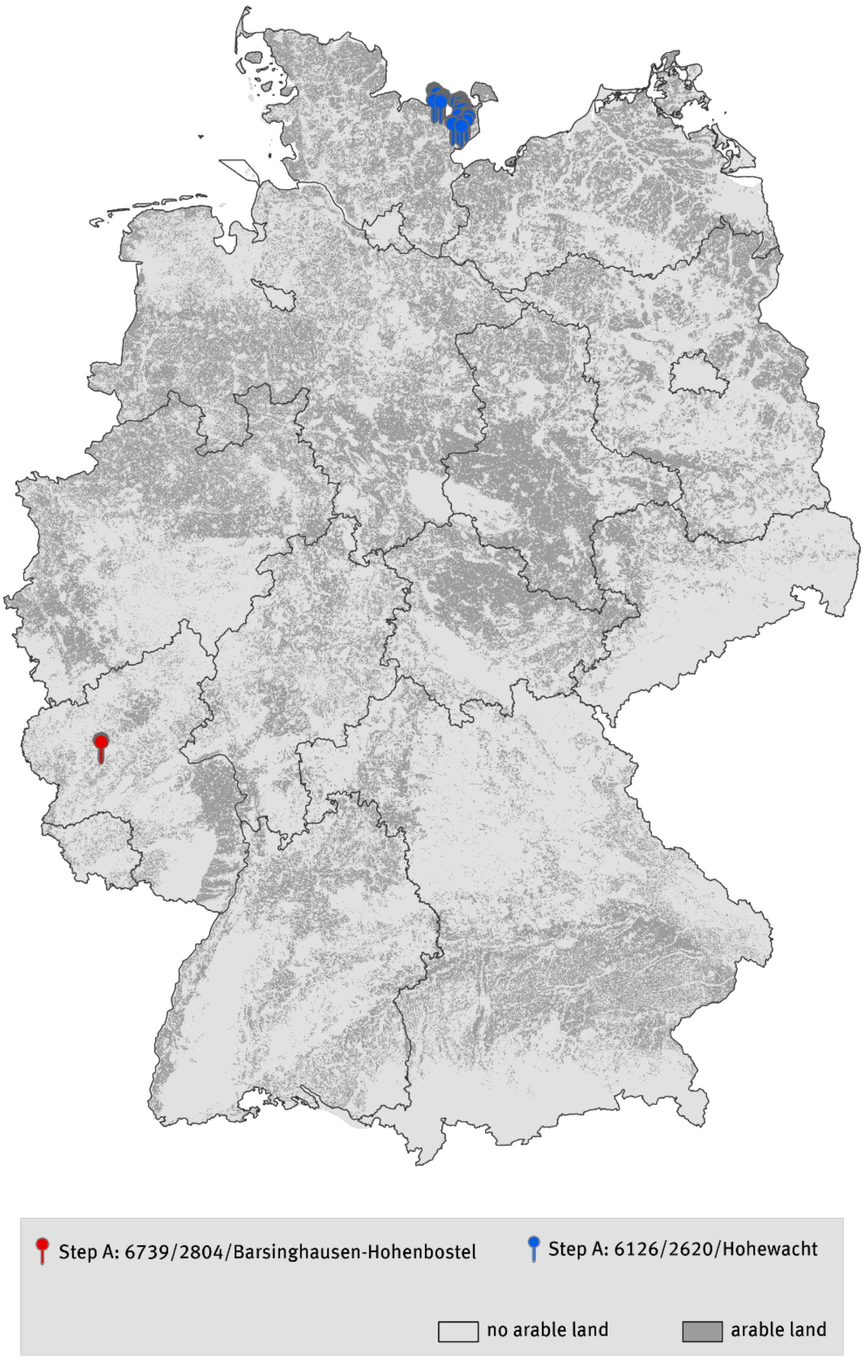
Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	30	1.99	0.24	0.09	0.87	1.0
2	10	2.05	0.22	0.09	0.29	0.5
3	10	1.81	0.31	0.16	0.2	0.5
4	30	1.81	0.31	0.16	0.2	0.3
5	20	1.84	0.3	0.15	0.1	0.3

Figure 88 shows the location and size of the two selected climate-soil scenarios. The scenario 6739/2804/Barsinghausen-Hohenbostel represents a small agricultural area of 2 km^2 with sandy soils in Southwest Germany. The geographical distance to the original weather station is rather large as the DWD station ‘Barsinghausen-Hohenbostel’ is located in Lower Saxony. However, it belongs to the same major hydrogeologic regions and was statistically selected as station with suitable weather conditions (Klein et al. 2019b). The scenario 6126/2620/Hohwacht represents an agricultural area of 24 km^2 with typical soils on glacial deposits and is located close the Fehmarn Island in East Schleswig-Holstein.

In Table 81 and Table 82 comparisons are provided between estimated percolate concentrations from the FOCUS Hamburg scenario, the two scenarios 6739/2804/Barsinghausen-Hohenbostel and 6126/2620/Hohwacht and the 80th spatial percentile from GeoPELMO DE (FOCUS L) as well as the spatial percentile, which concentrations from the scenarios represent. The results demonstrate that both selected climate-soil scenarios meet the requirements regarding the 80 ± 5th percentile for most of the active substances and transformation products. In few situations the estimated leaching concentrations represent a percentile above the 85th or below the 75th percentile. However, both scenarios seem to be suitable alternative scenarios for German groundwater risk assessment considering the FOCUS leaching approach based on chromatographic flow (European Commission 2014).

Figure 88: Location and size of selected scenarios based on the FOCUS modelling approach considering chromatographic flow

The climate-soil combinations in the map were selected from simulation runs with GeoPELMO DE (FOCUS L). They represent the highest possible number of overlaps in the range between the 75th and 85th spatial percentile of all 14 percolate concentration maps for active substances and metabolites (step A).



Source: own illustration, Fraunhofer IME.

Table 81: Comparison of estimated percolate concentrations in 1 m soil depth from the FOCUS Hamburg scenario, the 80th spatial percentile from GeoPELMO DE (FOCUS L) and the two scenarios 6739/2804/Barsinghausen-Hohenbostel and 6126/2620/Hohwacht

Fourteen Model simulations are conducted for three dummy active substances, two fictive metabolites formed from different active substances and applications in maize and winter cereals. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance and metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS Hamburg [µg/L]	GeoPELMO DE FOCUL L [µg/L]	6739/2804/ Barsinghausen-Hohenbostel [µg/L]	6126/2620/ Hohwacht [µg/L]
Maize	P1	30	10	0.005	0.022	0.022	0.034
Maize	P2	60	20	0.029	0.088	0.118	0.107
Maize	P3	240	80	0.057	0.205	0.1805	0.360
Winter cereals	P1	30	10	0.400	0.932	1.1882	0.977
Winter cereals	P2	60	20	0.328	0.569	0.555	0.744
Winter cereals	P3	240	80	0.137	0.381	0.359	0.574
Maize	M2 (P1)	30	80	7.885	10.740	10.919	11.083
Maize	M1 (P2)	10	40	3.583	4.870	4.446	4.732
Maize	M2 (P2)	30	80	4.506	5.950	6.175	6.110
Maize	M2 (P3)	30	80	11.940	14.655	14.862	15.250
Winter cereals	M2 (P1)	30	80	18.290	19.941	19.427	20.997
Winter cereals	M1 (P2)	10	40	7.490	7.260	7.600	7.360
Winter cereals	M2 (P2)	30	80	7.650	8.780	8.670	8.902
Winter cereals	M2 (P3)	30	80	13.810	16.507	16.209	16.522

Table 82: **Comparison of the spatial percentile for estimated percolate concentrations in 1 m soil depth from the FOCUS Hamburg scenario and the two scenarios 6739/2804/Barsinghausen-Hohenbostel and 6135/2620/Hohwacht with the 80th spatial percentile from GeoPELMO DE (FOCUS L)**

Fourteen Model simulations are conducted for three dummy active substances, two fictive metabolites formed from different active substances and applications in maize and winter cereals. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance and metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS Hamburg [%]	GeoPELMO DE FOCUL L [%]	6739/2804/ Barsinghausen-Hohenbostel [%]	6126/2620/ Hohwacht [%]
Maize	P1	30	10	51.8	80.0	80.0	>85*
Maize	P2	60	20	59.1	80.0	84.1	82.2
Maize	P3	240	80	59.6	80.0	78.3	>85*
Winter cereals	P1	30	10	64.0	80.0	83.4	81.2
Winter cereals	P2	60	20	70.3	80.0	79.5	84.5
Winter cereals	P3	240	80	62.4	80.0	79.3	>85*
Maize	M2 (P1)	30	80	43.1	80.0	81.4	82.5
Maize	M1 (P2)	10	40	50.7	80.0	<75*	77.3
Maize	M2 (P2)	30	80	53.4	80.0	83.4	82.9
Maize	M2 (P3)	30	80	66.2	80.0	80.9	83.9
Winter cereals	M2 (P1)	30	80	74.1	80.0	78.3	84.9
Winter cereals	M1 (P2)	10	40	82.6	80.0	83.4	81.6
Winter cereals	M2 (P2)	30	80	71.6	80.0	78.1	81.3
Winter cereals	M2 (P3)	30	80	69.8	80.0	78.4	80.0

* estimated values

6.1.3 Scenarios considering chromatographic and preferential flow, runoff and drainage

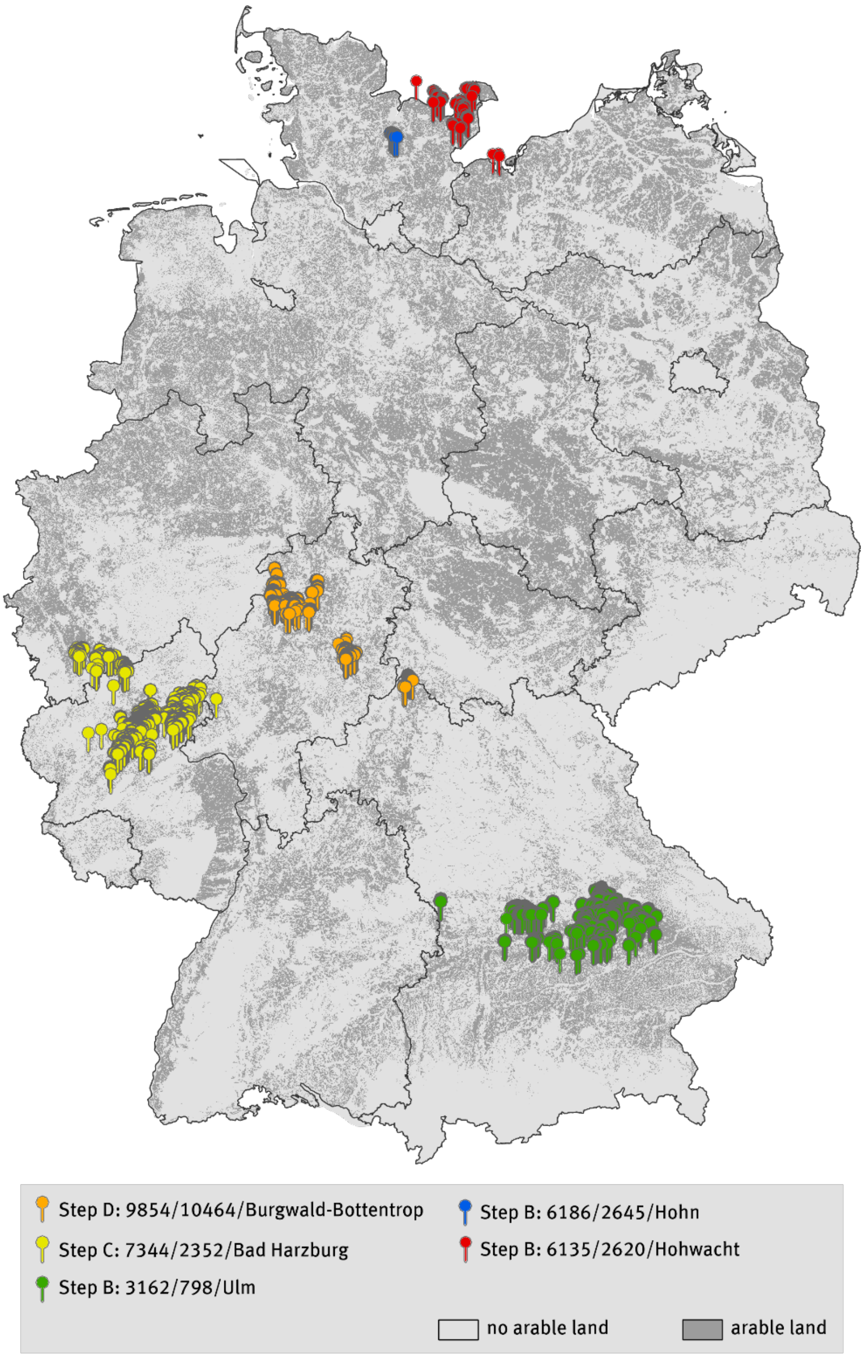
Three realistic worst-case scenarios were selected with reference to the methodological **step B** (maximum number of possible overlaps of the 75th to 85th spatial percentile from all 14 percolate concentration maps) described in chapter 6.1.1. All simulation runs are conducted with GeoPELMO DE (FOCUS L+R+M+D) considering chromatographic and preferential flow, runoff and drainage. Finally, no area with an overlap of all 14 concentration maps exists. Therefore, two climate-soil-scenarios with number 6135, soil profile number 2620 and weather station 'Hohwacht' (ID: 6135/2620/Hohwacht) and with number 6186, soil profile number 2645 and weather station 'Ulm' (6186/2645/Hohn) represent the highest possible number of 13 overlaps. The 75th-85th percentiles of the concentration map for active substance P1 in maize is not covered with scenario 6135/2620/Hohwacht. And the climate-soil-scenario with number 3162, soil profile number 798 and weather station 'Ulm' (3162/798/Ulm) represents 11 overlaps of all 14 percolate concentration maps including P1 in maize. In Figure 89, the location and size of the selected scenarios is shown. An overview of typical properties of the three selected scenarios is presented in Table 83.

Table 83 and Table 84 provide depth dependent soil properties as parameterised in GeoPELMO DE. Overall, the two soil profiles from scenarios 6186/2645/Hohn and 6135/2620/Hohwacht are rather similar. However, soil profile 2645 is exceptional since the second horizon is characterised by a higher organic carbon content than the top soil layer. It is recommended to consider the climate station Hohwacht together with BÜK soil profile 2620 as alternative scenario, because the representativeness of the combination 6186/2645/Hohn is lower than for the combination 6135/2620/Hohwacht.

Table 86 and Table 87 show modelling results for all 14 compound/crop combinations. The percolate concentrations are in the range of 80 ± 5% in 13 of 14 simulation runs with scenario 6135/2620/Hohwacht. shows PELMO results for all 14 compound/crop combinations using combination 3162. And the percolate concentrations are in the range of 80 ± 5% in 11 of 14 simulation runs with scenario 3162/798/Ulm.

Figure 89: Location and size of selected scenarios based on the spatial distributed modelling considering chromatographic and preferential flow, runoff and drainage (step B-D)

The climate-soil combinations in the map were selected from simulation runs with GeoPELMO DE (FOCUS L+R+M+D). They represent the highest possible number of overlaps in the range between the 75th and 85th spatial percentile of all 14 percolate concentration maps for active substances and metabolites (step B), of all 6 percolate concentration maps for active substances (step C) and of all 8 percolate concentration maps for metabolites (step D).



Source: own illustration, Fraunhofer IME.

Table 83: **Properties of climate-soil combinations from selection step B**

Combination No.	6135 (6126^)	6186	3162
Soil number	2620	2645	798
Weather station	Hohwacht	Hohn	Ulm
Average annual precipitation (mm)	698	821	736
Average annual air temperature (°C)	9.3	8.9	8.6
Soil description (in German)	Parabraunerden mit Pseudogleyen aus Geschiebelehm über (tiefem) Geschiebemergel vergesellschaftet mit Pararendzinen aus Geschiebemergel	Podsole mit Pseudogley-Podsolen aus Flugsand oder Decksand über Geschiebelehm	Braunerden aus Lösslehm über tiefer Lehmfließerde oder Sand aus Molasse (-verwitterung)
Organic carbon content, top soil/0-1 m (%)	0.87/0.37	0.87/0.44	0.87/0.45
Average clay/silt/sand content (%)	17/35/48	11/25/64	20/36/44
Macropore class	2 (moderate)	2 (moderate)	2 (moderate)
Drainage	no	no	no
Runoff	yes	yes	yes
Selection Step	B	B	B
Number of overlaps for active substances (maximum 6) and metabolites (max. 8)	13	13	11*
Agricultural area (km²)	6.5	1.6	97

^ Combination number 6126 changes to number 6135 if drainage is included in GeoPELMO DE (FOCUS L+R+M+D)

* No matches for active substance P1 in winter cereals and metabolite M1 formed from P2 and P1 in winter cereals

Table 84: **Detailed information for soil profile 2645 (used in combination 6186)**

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	30	1.99	0.24	0.09	0.87	1.0
2	5	1.89	0.22	0.09	1.74	0.5
3	15	2.05	0.31	0.09	0.2	0.5
4	20	2.05	0.31	0.09	0.2	0.3
5	30	1.99	0.3	0.11	0.1	0.3

Table 85: Detailed information for soil profile 798 (used in combination 3162)

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	30	1.99	0.24	0.09	0.87	1.0
2	5	1.89	0.22	0.09	1.74	0.5
3	15	2.05	0.31	0.09	0.2	0.5
4	20	2.05	0.31	0.09	0.2	0.3
5	30	1.99	0.3	0.11	0.1	0.3

Table 86: Comparison of estimated percolate concentrations in 1 m soil depth and spatial percentiles from the FOCUS Hamburg scenario, the 80th spatial percentile from GeoPELMO DE (FOCUS L+R+M+D) and the selected scenario 6135/2620/Hohwacht

Fourteen Model simulations are conducted for three dummy active substances, two fictive metabolites formed from different active substances and applications in maize and winter cereals. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance and metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS Hamburg [µg/L]	GeoPELMO DE FOCUL L+R+M+D [µg/L]	6135/2620/ Hohwacht [µg/L]	6135/2620/ Hohwacht [%]
Maize	P1	30	10	0.005	0.055	0.041	<75 (estimated)
Maize	P2	60	20	0.029	0.146	0.123	75.8
Maize	P3	240	80	0.057	0.257	0.313	84.2
Winter cereals	P1	30	10	0.400	0.895	0.695	75.5
Winter cereals	P2	60	20	0.328	0.626	0.790	84.8
Winter cereals	P3	240	80	0.137	0.412	0.528	84.2
Maize	M2 (P1)	30	80	7.890	10.341	10.798	83.3
Maize	M1 (P2)	10	40	3.580	4.810	4.514	77.2
Maize	M2 (P2)	30	80	4.510	5.648	6.022	84.2
Maize	M2 (P3)	30	80	11.94	13.955	14.855	84.0
Winter cereals	M2 (P1)	30	80	18.29	20.109	20.883	82.6
Winter cereals	M1 (P2)	10	40	7.490	7.525	7.197	77.1
Winter cereals	M2 (P2)	30	80	7.650	8.784	9.061	82.0
Winter cereals	M2 (P3)	30	80	13.810	16.387	15.745	78.0

Table 87: Comparison of estimated percolate concentrations in 1 m soil depth and spatial percentiles from the FOCUS Hamburg scenario, the 80th spatial percentile from GeoPELMO DE (FOCUS L+R+M+D) and the selected scenario 3162/798/Ulm

Fourteen Model simulations are conducted for three dummy active substances, two fictive metabolites formed from different active substances and applications in maize and winter cereals. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance and metabolite	K_{foc} {L/kg]	$DegT_{50}$ {d]	FOCUS Hamburg {µg/L]	GeoPELMO DE FOCUL L+R+M+D {µg/L]	3162/798/ Ulm {µg/L]	3162/798/ Ulm {%]
Maize	P1	30	10	0.005	0.055	0.066	83.9
Maize	P2	60	20	0.029	0.146	0.149	80.8
Maize	P3	240	80	0.057	0.257	0.231	77.0
Winter cereals	P1	30	10	0.400	0.895	0.432	< 70*
Winter cereals	P2	60	20	0.328	0.626	0.555	77.4
Winter cereals	P3	240	80	0.137	0.412	0.397	79.2
Maize	M2 (P1)	30	80	7.890	10.341	10.179	78.0
Maize	M1 (P2)	10	40	3.580	4.810	3.391	<70*
Maize	M2 (P2)	30	80	4.510	5.648	5.770	81.4
Maize	M2 (P3)	30	80	11.94	13.955	14.669	83.5
Winter cereals	M2 (P1)	30	80	18.290	20.109	20.994	83.0
Winter cereals	M1 (P2)	10	40	7.490	7.525	6.969	<75*
Winter cereals	M2 (P2)	30	80	7.650	8.784	9.230	83.7
Winter cereals	M2 (P3)	30	80	13.810	16.387	17.235	84.5

* estimated

The alternative scenarios selected based on of the highest possible number of overlaps of all 14 percolate concentration maps (step B according to chapter 6.1.1) were not representative for the 80 ± 5 spatial percentiles of all dummy active substances considered in the simulations. Therefore, a reduced search for alternative scenarios was performed for all dummy active substances P1, P2, P3 applied in maize and winter cereals (**step C**). In total, 27 climate-soil combinations fulfilled that requirement. In all those combinations, macropore flow is one of the dominant processes. The scenario with the maximum coverage was combination number 7344 with soil profile number 2352 and the DWD weather station Bad Harzburg (ID: 7344/2352/Bad Harzburg).

The same approach was conducted for metabolites. To find more appropriate scenarios for the transformation products a reduced search was performed for dummy metabolites M1 and M2 formed from different active substances after application in maize and winter cereals (**step D**). In total, 16 climate-crop combinations fulfilled a maximum of overlaps. In the previous selections, only scenarios were identified with macropore flow. In contrast, the selected scenario for the metabolites, which a maximum coverage of agricultural area, are soils without macropore flow parametrisation. This scenario is represented by combination number 9854 with soil profile number 10464 and DWD weather station 'Burgwald-Bottendorf' (ID: 9854/10464/Burgwald-Bottendorf).

In Figure 89, the location and size of both scenarios 7344/2352/Bad Harzburg and 9854/ 10464/Burgwald-Bottendorf from selection step C and step D are shown. Their properties are presented in Table 88. An overview of typical properties is provided in Table 89 and Table 90.

Table 88: Properties of two climate-soil combinations from selection step C and D

Combination No.	7433	9854
Soil number	2352	10464
Weather station	Bad Harzburg	Burgwald-Bottendorf
Average annual precipitation (mm)	773	684
Average annual air temperature (°C)	9.2	8.6
Soil description (in German)	Braunerden mit Regosolen aus Schluff- oder Lehmfließerde über Grus- oder Schuttlehmfließerde aus Tonschiefer (Tongestein)	Braunerden mit Podsol-Braunerden aus Sandfließerde oder grusigem Verwitterungs-sand über Schuttsand- oder Lehmschuttfließerde aus Sandstein-Schluffstein-Wechselfolgen
Organic carbon content, topsoil/0-1 m (%)	1.74/0.61	1.74/0.55
Average clay/silt/sand content (%)	33/56/11	8/21/71
Macropore class	3 (high macropore flow)	1 (no macropore flow)
Drainage	no	no
Runoff	yes	yes
Selection step	C	D
Number of overlaps for active substances (maximum 6)	6	-
Number of overlaps for metabolites (maximum 8)	-	8
Agricultural area (km²)	75	62

Table 89: Detailed information for soil profile 2352 (used in combination 7344)

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	30	1.63	0.38	0.18	1.74	1.0
2	20	1.68	0.36	0.25	0.2	0.5
3	50	1.68	0.36	0.25	0.1	0.3

Table 90: Detailed information for soil profile 10464 (used in combination 9854)

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	25	1.89	0.28	0.09	1.74	1.0
2	5	2.05	0.22	0.09	0.2	1.0
3	20	2.05	0.22	0.09	0.2	0.5
4	50	2.15	0.18	0.06	0.1	0.3

Table 91 shows a comparison between estimated percolate concentrations from the FOCUS Hamburg scenario, the scenario 7344/2352/Bad Harzburg and the 80th spatial percentile from GeoPELMO DE (FOCUS L+R-M+D) as well as the spatial percentile, which it represents. As expected, the results for this combination are within the range of the 80 ± 5th spatial percentiles for the dummy active substances. However, all modelling results for the metabolites are significantly below the targeted 80th spatial percentile. This is probably caused by intensive macropore flow in this climate-soil combination, which leads to fast leaching of the active substance to deeper soil layers, and significant lower amounts are available in the soil profile to be transformed to metabolites M1 or M2.

Table 92 shows a comparison between estimated percolate concentrations from the FOCUS Hamburg scenario, the scenario 9854/10464/Burgwald-Bottendorf and the 80th spatial percentile from GeoPELMO DE (FOCUS L+R-M+D) as well as the spatial percentile, which the scenario represents. As expected, the results for this combination are within the range of 80 ± 5th spatial percentile for the transformation products. However, all results for the active substances are significantly below the targeted 80th spatial percentile. This was probably the case because the algorithm picked locations with high potential of metabolite formation in the soil profile, which cannot be a realistic worst-case situation for the leaching of the precursor active substance at the same time. However, the modelled percolate concentrations of this scenario are above the results of respective FOCUS Hamburg simulations.

Table 91: Comparison estimated percolate concentrations in 1 m soil depth and spatial percentiles from the FOCUS Hamburg scenario, the 80th spatial percentile from GeoPELMO DE (FOCUS L+R+M+D) and the selected scenario 7344/2352/Bad Harzburg

Fourteen Model simulations are conducted for three dummy active substances, two fictive metabolites formed from different active substances and applications in maize and winter cereals. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance and metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS Hamburg [µg/L]	GeoPELMO DE FOCUL L+R+M+D [µg/L]	7344/2352/ Bad Harzburg [µg/L]	7344/2352/ Bad Harzburg [%]
Maize	P1	30	10	0.005	0.055	0.062	82.6
Maize	P2	60	20	0.029	0.146	0.171	84.4
Maize	P3	240	80	0.057	0.257	0.262	80.4
Winter cereals	P1	30	10	0.400	0.895	0.729	76.6
Winter cereals	P2	60	20	0.328	0.626	0.628	80.2
Winter cereals	P3	240	80	0.137	0.412	0.405	79.6
Maize	M2 (P1)	30	80	7.890	10.341	6.320	<40*
Maize	M1 (P2)	10	40	3.580	4.810	2.380	<30*
Maize	M2 (P2)	30	80	4.510	5.648	3.390	<40*
Maize	M2 (P3)	30	80	11.940	13.955	8.575	<40*
Winter cereals	M2 (P1)	30	80	18.290	20.109	13.463	<50*
Winter cereals	M1 (P2)	10	40	7.490	7.525	5.623	<60*
Winter cereals	M2 (P2)	30	80	7.650	8.784	4.464	<30*
Winter cereals	M2 (P3)	30	80	13.810	16.387	10.032	<40*

* estimated

Table 92: Comparison of estimated percolate concentrations in 1 m soil depth and spatial percentiles from the FOCUS Hamburg scenario, the 80th spatial percentile from GeoPELMO DE (FOCUS L+R+M+D) and the selected scenario 9854/10464/Burgwald-Bottendorf

Fourteen Model simulations are conducted for three dummy active substances, two fictive metabolites formed from different active substances and applications in maize and winter cereals. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance and metabolite	K_{foc} [L/kg]	$DegT_{50}$ [d]	FOCUS Hamburg [µg/L]	GeoPELMO DE FOCUL L+R+M+D [µg/L]	9854/10464/ Burgwald-Bottendorf [µg/L]	9854/10464/ Burgwald-Bottendorf [%]
Maize	P1	30	10	0.005	0.055	0.008	<30*
Maize	P2	60	20	0.029	0.146	0.047	<45*
Maize	P3	240	80	0.057	0.257	0.083	<45*
Winter cereals	P1	30	10	0.400	0.895	0.708	<75*
Winter cereals	P2	60	20	0.328	0.626	0.312	<65*
Winter cereals	P3	240	80	0.137	0.412	0.176	<65*
Maize	M2 (P1)	30	80	7.890	10.341	10.185	78.0
Maize	M1 (P2)	10	40	3.580	4.810	4.769	79.7
Maize	M2 (P2)	30	80	4.510	5.648	5.728	80.9
Maize	M2 (P3)	30	80	11.940	13.955	13.388	76.9
Winter cereals	M2 (P1)	30	80	18.290	20.109	18.844	75.6
Winter cereals	M1 (P2)	10	40	7.490	7.525	7.168	77.0
Winter cereals	M2 (P2)	30	80	7.650	8.784	8.302	76.9
Winter cereals	M2 (P3)	30	80	13.810	16.387	15.187	76.3

* estimated

In addition to the selection **steps B, C, D** based on the most possible overlaps, seven further selection steps (**steps E-L**) were carried out in order to consider different substance properties or different application period in the search for representative scenarios for Germany (see chapter 6.1.1, Figure 85). The location and size of seven selected alternative scenarios is provided in Figure 90. An overview of typical properties of the three selected scenarios is presented in Table 93. Table 85, Table 89, Table 94 to Table 98 provide depth dependent soil properties as parameterised in GeoPELMO DE.

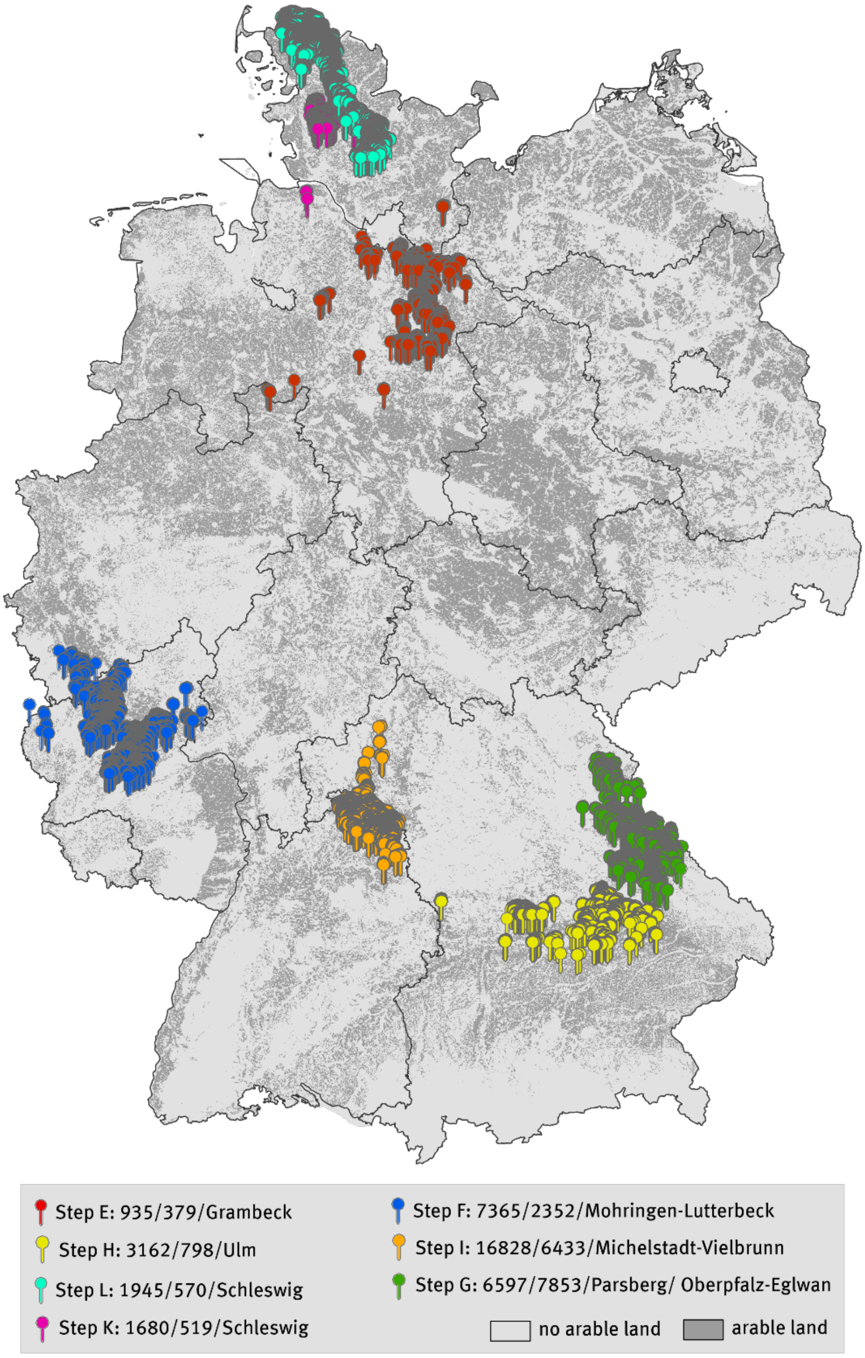
In **step E** and **step F**, two scenarios were selected for different application times independent of active substance properties. The climate-soil-scenario with number 935, soil profile number 379 and DWD weather station 'Grambek' (ID: 935/379/Grambek) represents the targeted spatial percentiles for active substances and applications in spring/summer (maize, step E), while the climate-soil-scenario with number 7365, soil profile number 2352 and weather station 'Moringen-Lutterbeck' (ID: 7365/2352/Moringen-Lutterbeck) represents the targeted spatial percentiles for active substances and applications in autumn/winter (winter cereals, step F).

The same was done in **step K** and **step L** for metabolites. The climate-soil-scenario with number 1680, soil profile number 519 and weather station 'Schleswig' (ID: 1680/519/Schleswig) represents the targeted spatial percentiles for metabolites and applications in spring/summer (maize, step K). In contrast, the climate-soil-scenario with number 1945, soil profile number 570 and with weather station 'Schleswig' (ID: 1945/570/Schleswig) represents the targeted spatial percentiles for metabolites and applications in in autumn/winter (winter cereals, step L).

In **step G**, **step H** and **step I**, the selection is conducted to find rather climate-soil combinations which represent different active substance properties and are independent from seasonal application times. The climate-soil-scenario with number 6597, soil profile number 7853 and weather station 'Parsberg/Oberpfalz-Eglwan' (ID: 6597/7853/Parsberg/Oberpfalz-Eglwan) represents the targeted spatial percentiles for fast degrading and very mobile dummy active substance P1 (**step G**). The climate-soil-scenario with number 3162, soil profile number 798 and weather station 'Ulm' (ID: 3162/798/Ulm) represents the targeted spatial percentiles for fast degrading and moderate mobile dummy active substance P2 (**step H**). The climate-soil-scenario with number 16828, soil profile number 6433 and weather station 'Michelstadt-Vielbrunn' (ID: 16828/6433/Michelstadt-Vielbrunn) represents the targeted spatial percentiles for moderate degrading and less mobile dummy active substance P3 (**step I**).

Figure 90: Location and size of selected scenarios based on the spatial distributed modelling considering chromatographic and preferential flow, runoff and drainage (step E-L)

The climate-soil combinations in the map were selected from simulation runs with GeoPELMO DE (FOCUS L+R+M+D). They represent overlaps in the range between the 75th and 85th spatial percentile by considering different compound properties (steps G, H, I) or different application period (steps E, F, K, L).



Source: own illustration, Fraunhofer IME.

Table 93: **Properties of seven climate-soil combinations from selection step E-to L**

Combination No.	**935**	**7365**	**6597**	**16828**	**1680**	**1945**
Soil number	379	2352	7853	6433	519	570
Weather Station	Grambek	Moringen-Lutterbeck	Parsberg/ Oberpfalz-Eglwan	Michelstadt-Vielbrunn	Schleswig	Schleswig
Average annual precip. (mm)	743	843	842	835	856	856
Average annual air temp. (°C)	9.0	n.a.	8.1	n.a.	8.8	8.8
Soil description (in German)	Braunerden, Podsol-Braunerden und Braunerde Podsole aus Decksand oder Flugsand über Schmelzwassersand	Braunerden mit Regosolen aus Schluff- oder Lehmfließerde über Grus- oder Schuttlehmfließerde aus Tonschiefer (-gestein)	Braunerden aus Decksand oder -lehm über (tiefem) grusigem/ steinigem Sand aus Granit oder Gneis	Braunerde-Pelosole und Braunerde-Terra fuscen mit Parabraunerden aus toniger Deckschicht oder aus Lösslehm und Pararendzinen mit Rendzinen aus (carbonathaltigem) Schuttlehm oder -ton über Carbonatgestein	Pseudogleye mit Pseudogley-Braunerden und Braunerden über Parabraunerde aus Decksand über (tiefem) Geschiebelehm	Podsole und Gley-Podsole aus Flugsand über Sandersand vergesellschaftet mit Braunerden aus Geschiebedecksand über Sandersand
Org. carbon, top soil/0-1 m (%)	0.87/0.38	1.74/0.61	1.74/0.66	1.74/0.64	0.87/0.36	1.74/0.60
Average clay/ silt/sand (%)	3/12/86	33/56/11	13/24/62	50/32/18	16/30/55	3/5/93
Macropore class	1	3	2	3	2	1
Drainage	no	no	no	no	no	yes
Runoff	yes	yes	yes	yes	yes	yes
Selection step	E	F	G	I	K	L
No. of overlaps for a.s. (max. 6)	3	3	2	2	-	-
No. of overlaps for met. (max. 8)	-	-	-	-	4	4
Agric. area (km²)	142	76	239	177	62	456

^ Properties of scenario with ID 3162/798/Ulm from selection step B and step H are already provided in

Table 83 and Table 85.

Table 94: Detailed information for soil profile 379 (used in combination 935)

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	30	2.1	0.2	0.05	0.87	1.0
2	20	2.18	0.17	0.05	0.29	0.5
3	5	2.18	0.17	0.05	0.29	0.3
4	45	2.31	0.12	0.02	0.1	0.3

Table 95: Detailed information for soil profile 7853 (used in combination 6597)

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	25	1.63	0.28	0.11	1.74	1.0
2	5	1.68	0.24	0.11	0.29	1.0
3	20	1.68	0.24	0.11	0.29	0.5
4	10	1.63	0.24	0.11	0.29	0.3
5	30	1.68	0.24	0.11	0.29	0.3
6	10	1.68	0.17	0.05	0.1	0.3

Table 96: Detailed information for soil profile 6433 (used in combination 16828)

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	30	1.63	0.38	0.25	1.74	1.0
2	20	1.63	0.38	0.29	0.2	0.5
3	30	1.63	0.38	0.29	0.2	0.3
3	20	1.63	0.38	0.29	0.1	0.3

Table 97: Detailed information for soil profile 519 (used in combination 1680)

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	30	1.99	0.24	0.09	0.87	1.0
2	20	2.05	0.22	0.09	0.2	0.5
3	50	1.84	0.3	0.15	0.1	0.3

Table 98: Detailed information for soil profile 570 (used in combination 1945)

Horizon	Depth [cm]	Density [kg/L]	Field capacity [cm³/cm³]	Wilting point [cm³/cm³]	OC content [%]	Degradation factor [-]
1	25	2.07	0.21	0.03	1.74	1.0
2	5	2.2	0.16	0.03	0.29	1.0
3	20	2.2	0.16	0.03	0.29	0.5
4	20	2.2	0.16	0.03	0.29	0.3
5	30	2.31	0.12	0.02	0.1	0.3

In most of the selected scenarios in step E-L soil profiles were identified where macropore flow was included as additional process. However, there are two climate-soil scenarios (combinations 935/379/Grambek and 1945/570/Schleswig) which represent larger agricultural areas and macropore flow is not considered (see Figure 88). Scenario 935/379/Grambek is interesting as it covers the national FOCUS Hamburg scenario whereas scenario 1945/570/Schleswig represents conditions in the centre of Schleswig-Holstein, very north of Germany. Table 99 shows, as an example, the performance of these two scenarios in relation to FOCUS Hamburg and the 80th spatial percentile calculated with GeoPELMO DE (FOCUS L+R+M+D).

It can be observed that the results of which spatial percentiles are finally covered by the selected scenarios for different crop-compound-applications very much depend on the respective overlapping rule. When, for example, only active substances in maize were considered for the overlapping strategy (step E: scenario 935/379/Grambek), only the results from the same simulation runs were found to be in the range of 80 ± 5 % compared to GeoPELMO DE. For all other crop-compound application runs concentrations outside the required range have been modelled with this single scenario, *i.e.* in this case a significantly higher percentiles than the 80th percentile have been met. In principle, the same outcome was found for the scenario 1945/570/Schleswig (selection step L mainly for metabolites in winter cereals. Metabolite concentrations were simulated close to 80 % even for applications in maize. However, the scenario did not meet the desired percentile for most active substances. The same results can be expected for the other selection steps F to K. If one scenario from an overlapping strategy includes only a certain number of crop-compound-situations, other crop-compound-situations would be expected to significantly lay outside the range of the 80 ± 5th percentile. This makes it finally difficult to find individual scenarios that are both representative and equally protective for active substances and metabolites with different properties and for different application periods and crops. A further limitation is that the scenarios derived in this chapter were based on a limited number of active substances and metabolites with fictitious properties, application periods and application rates. A much wider range of substance properties and application parameters must be expected for the assessment and authorisation of real intended uses of plant protection product. Therefore, an evaluation of the protection level of the selected scenarios is extended to active substances and metabolites of real plant protection product uses in the following chapter.

Table 99: Comparison of estimated percolate concentrations in 1 m soil depth and spatial percentiles from the FOCUS Hamburg scenario, the 80th spatial percentile from GeoPELMO DE (FOCUS L+R+M+D) and the selected scenarios 935/379/Grambek and 1945/570/Schleswig

Fourteen Model simulations are conducted for three dummy active substances, two fictive metabolites formed from different active substances and applications in maize and winter cereals. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Crop	Active substance and metabolite	FOCUS Hamburg [µg/L]	GeoPELMO DE FOCUL L+R+M+D [µg/L]	935/379/ Grambek [µg/L]	935/379/ Grambek [%]	1945/570/ Schleswig [µg/L]	1945/570/ Schleswig [%]
Maize	P1	0.005	0.055	0.536	79.1	0.020	45*
Maize	P2	0.029	0.146	0.165	83.6	0.045	40*
Maize	P3	0.057	0.257	0.296	83.1	0.088	<45*
Winter cereals	P1	0.400	0.895	2.480	>90*	0.965	82.2
Winter cereals	P2	0.328	0.626	1.380	>90*	0.405	70*
Winter cereals	P3	0.137	0.412	0.607	>85*	0.170	60*
Maize	M2 (P1)	7.890	10.341	12.751	95*	11.237	>85*
Maize	M1 (P2)	3.580	4.810	5.957	>90*	5.792	>90*
Maize	M2 (P2)	4.510	5.648	7.054	>90*	6.024	84.7
Maize	M2 (P3)	11.940	13.955	17.223	>90*	14.053	80.9
Winter cereals	M2 (P1)	18.290	20.109	22.327	>85*	18.906	76.1
Winter cereals	M1 (P2)	7.490	7.525	10.171	>90*	8.0969	84.7
Winter cereals	M2 (P2)	7.650	8.784	10.222	>90*	8.0304	75.6
Winter cereals	M2 (P3)	13.810	16.387	18.639	>90*	15.102	75.9

* estimated

6.2 Verification of national scenarios based on real pesticide uses

In the previous chapters artificial dummy active substances, transformation products and application patterns were used to analyse the current level of protection in groundwater risk assessment and to derive alternative scenarios for the national lower tier groundwater risk assessment. In chapter 6.2 the impact of eight new potential scenarios on the national groundwater risk assessment is analysed based on real pesticide uses. Consequences for a regulatory use of the new scenarios are theoretically discussed in comparison to the current lower tier risk assessment (FOCUS Hamburg scenario used as single scenario in the national groundwater risk assessment) and compared to modelling results from GeoPELMO DE. The idea behind is to evaluate in more detail the robustness of the proposed scenarios regarding their level of protection. In chapter 6.2.1 the pesticide uses considered and the range of properties of all active substances and their metabolites are provided. The spatial distributions of estimated percolate concentrations are discussed in chapter 6.2.2. The FOCUS Hamburg scenario and two new scenarios are validated in terms of their protection goal in chapter 6.2.3 for the model version of GeoPELMO DE (FOCUS L) considering chromatographic flow, only. FOCUS Hamburg and six scenarios are validated in chapter 6.2.4 for the model version of GeoPELMO DE (FOCUS L+R+M+D) considering chromatographic and preferential flow, runoff and drainage.

6.2.1 Pesticides use considered for the evaluation

A subset of real pesticide uses for 11 active substances and 34 selected metabolites are used for the evaluation of new potential groundwater scenarios, whereby some of the pesticides uses are not authorised in Germany anymore. Table 100provides an overview about the application pattern of the pesticides used for the evaluation. Degradation and sorption values of the real active substances and metabolites cover a wider range of fate properties compared to the dummy active substances and metabolites which have been originally used for scenario selection (Figure 91). The different properties of the 11 active substances and 34 metabolites lead to different leaching tendencies which can be expressed by the Groundwater Ubiquity Score (GUS) index according to Gustafson (1989) (Figure 92). The calculation of the GUS index is based on the sorption constant K_{foc} and the half-life $DegT_{50}$ of a pesticide, whereby application rates and timings as well as formation fractions for the metabolites, which additionally influence leaching, are not considered.

Groundwater Ubiquity Score Index

The Groundwater Ubiquity Score (GUS) is used as index to express the leaching tendencies for organic chemical compounds. Its calculation according to Gustafson (1989) is based on the following equation:

$$\text{Groundwater Ubiquity Score (GUS)} = \text{Log}_{10}(DegT_{50}) \times [4 - \text{Log}_{10}(K_{foc})]$$

$DegT_{50}$: Degradation half-life (d)
K_{foc}: Sorption constant related to organic carbon in soil (L/kg):

The tendency to leach is summarised in three classes:

< 1.8: low potential for leaching

1.8-2.8: moderate potential for leaching

> 2.8: high potential for leaching

Table 100: Pesticide uses for the evaluation of new scenarios based on GeoPELMO DE (FOCUS L+R+M+D)

Fourteen Model simulations are conducted for three dummy active substances, two fictive metabolites formed from different active substances and applications in maize and winter cereals. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).

Active substance	Number of metabolites considered [-]	Target crop [-]	Application season [-]	Nominal application rate [kg/ha]	Growth stage (BBCH) [-]	Crop interception [%]
S-Metolachlor	7	maize	spring	1 x 1.250	< 9	0
Isoproturon	4	winter cereals	autumn	1 x 1.500	< 9	0
Diflufenican	2	winter cereals	autumn	1 x 0.1875	< 9	0
Chlorothalonil	3	winter cereals	spring	2 x 0.750	1 x 30 1 x 40	1 x 80 1 x 90
Bentazone	1	spring cereals	spring	1 x 0.960	12	0
Terbuthylazine	5	maize	spring	1 x 0.750	< 9	0
Clothianidin	3	sugar beet	spring	1 x 0.013	0	0°
Azoxystrobin	1	winter cereals	spring	2 x 0.250	> 32	80
Metazachlor	4	winter OSR	autumn	1 x 0.750	< 9	0
Flufenacet	2	winter cereals	autumn	1 x 0.240	10	0
Imazamox	2	winter OSR	autumn	1 x 0.0125	12	0

° incorporation in soil at 2.5 cm (seed treatment)

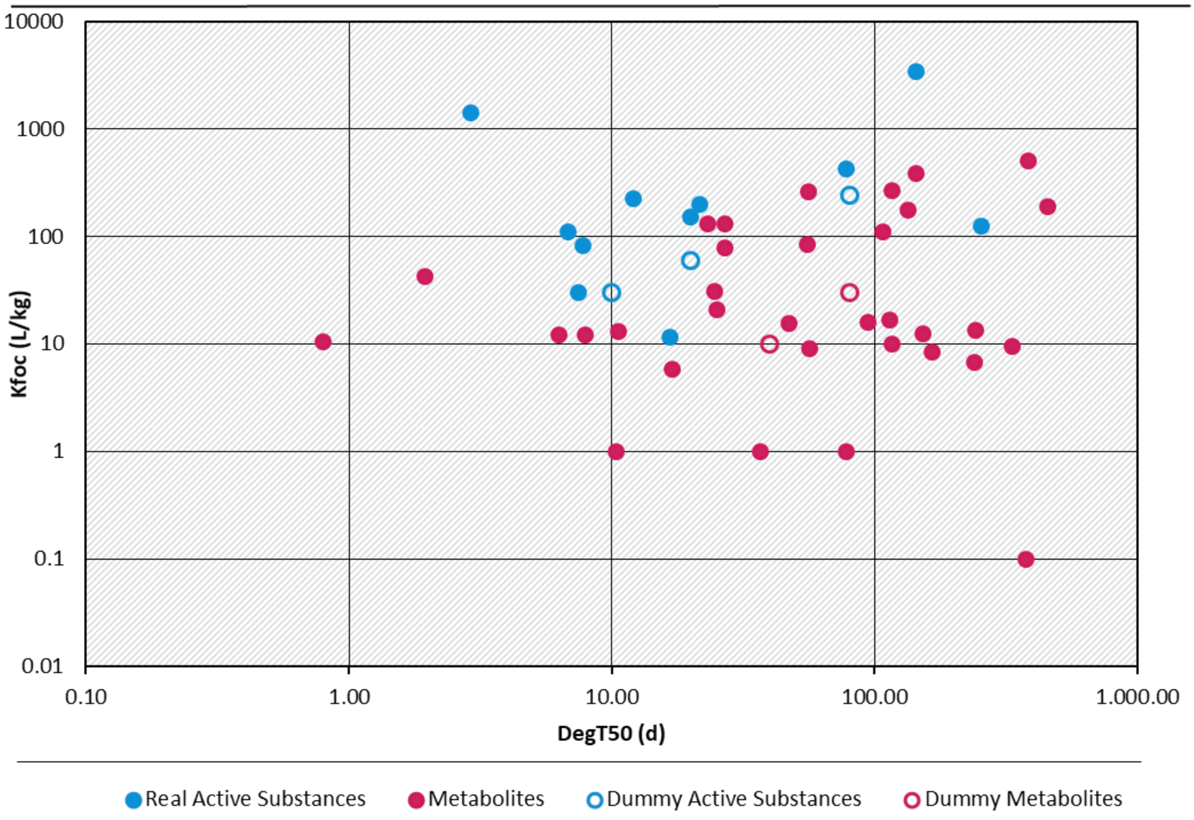
The GUS values in Figure 91 demonstrate a wide range from 0.4 (chlorothalonil, low potential for leaching) to 4.6 (clothianidin, high potential for leaching) for the active substances. This range is larger than the variability of the GUS values for the artificial parent compounds P1 (2.4), P2 (4.6) and P3 (3.0). More active substances with a lower tendency to leach are included in the verification of the new scenarios.

The variability of GUS indices for 34 real transformation products is even higher and ranges from -0.3 (metabolite CGA 37735 from S-metolachlor, low potential for leaching) to 24 (metabolite TFA from flufenacet, high potential for leaching). Compared to the two artificial dummy metabolites M1 (4.0) and M2 (4.7) a much wider range of GUS values, and thus a combination of degradation and sorption values, is covered in the analysis. For quite a lot of metabolites, the GUS values (and thus the tendency to leach) tend to be higher than for the active substances.

In Appendix D a detailed overview about the properties of the simulated active substances and metabolites is provided.

Figure 91: Properties of simulated active substances and metabolites

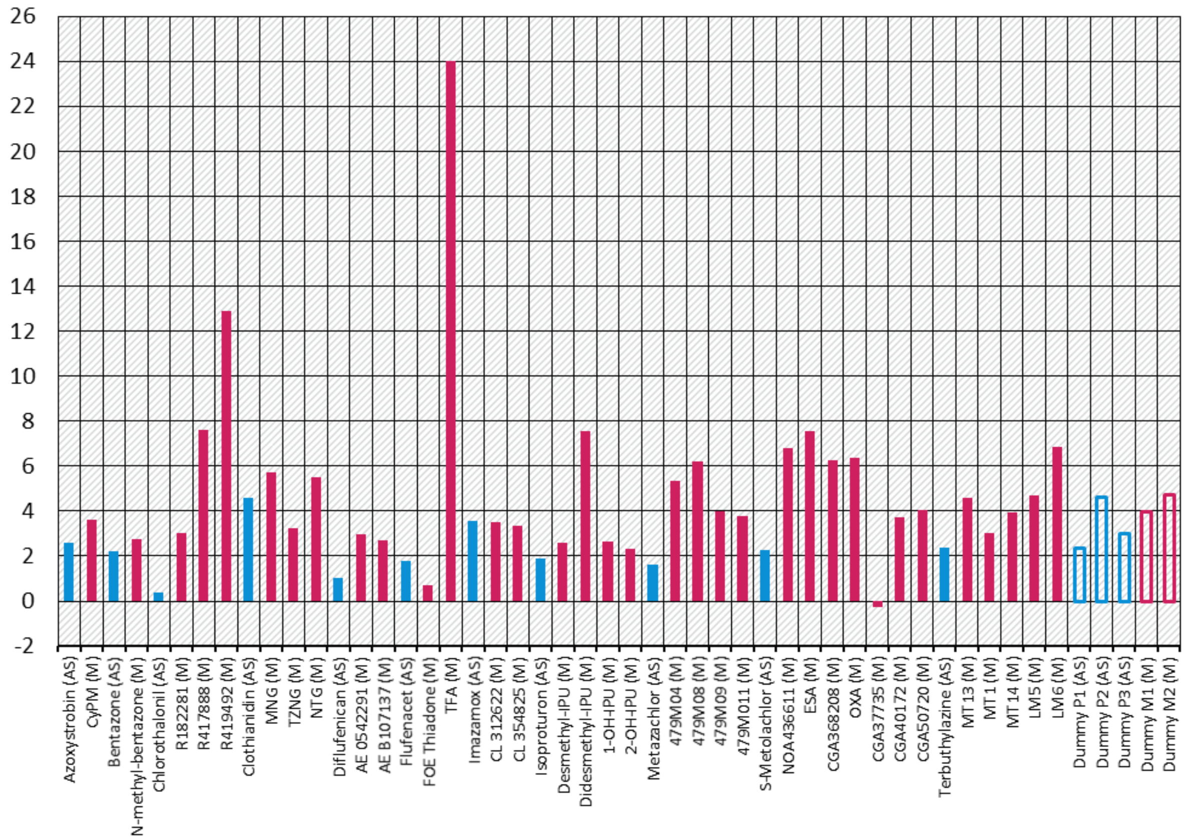
Normalised degradation ($DegT_{50}$) and sorption values (K_{foc}) of 11 real active substances and 34 selected metabolites are used for the scenario evaluation. For comparison, the properties of 3 dummy active substances and 2 metabolites according to chapter 5.1 are additionally provided in the diagram.



Source: own illustration, Fraunhofer IME.

Figure 92: Groundwater Ubiquity Score (GUS) of simulated active substances and metabolites

The calculated GUS values for 11 real active substances and 34 metabolites are in a range between -0.3 and 24. This range is larger than for the dummy active substances P1-P3 and metabolites M1-M2. The GUS values (and thus the tendency to leach) tend to be higher for the metabolites than for the active substances. The highest value was calculated for metabolite TFA.



$$\textit{Groundwater Ubiquity Score (GUS)} = \mathrm{Log}_{10}\,(\mathrm{DegT}_{50}) \times [4 - \mathrm{Log}_{10}\,(\mathrm{K}_{foc})]$$

Source: own illustration, Fraunhofer IME.

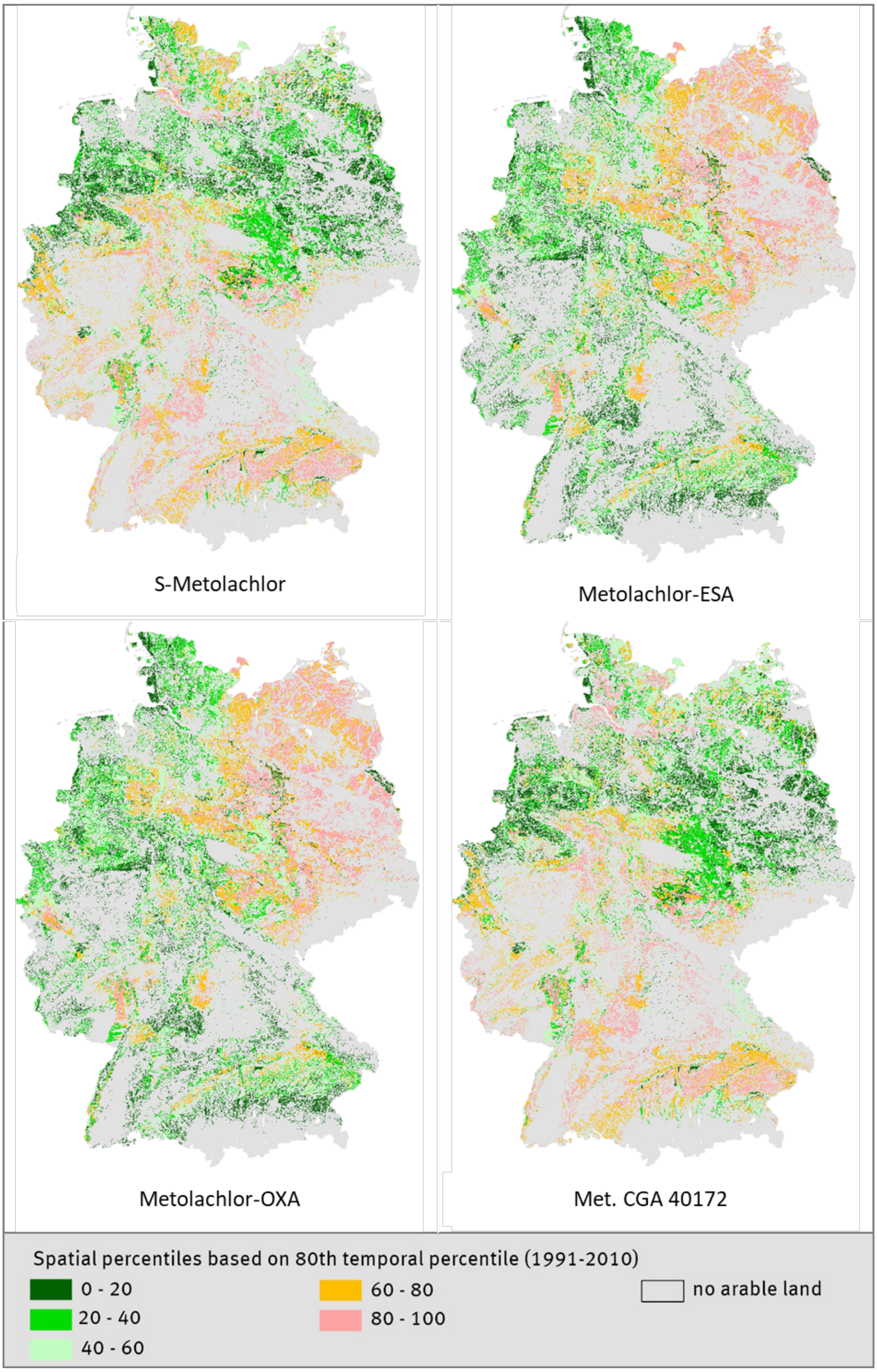
6.2.2 Spatial distribution of percolate concentrations

Three of eleven active substances and nine of their transformation products (metabolites) were selected and mapped with regard to the spatial distribution of annual percolate concentrations based on the GeoPELMO DE (FOCUS L+R+M+D) version considering chromatographic and preferential flow, runoff and drainage.

The maps for S-metolachlor and the three metabolites metolachlor-ESA, metolachlor-OXA and CGA 40172 illustrate one of the major outcomes of the previous chapters (Figure 93). Various processes in the PELMO model and the variability of fate properties (e.g. degradation, sorption, formation fraction) lead to different percolate concentration pattern for the different compounds. It is finally difficult to find a region (or a scenario) which represents the same spatial percentile for the active substance S-metolachlor and its metabolites. The nationwide distribution of concentration percentiles for the parent compound S-metolachlor is significantly different compared to two of its transformation products. While high concentrations of the active substance were calculated primarily in parts of Schleswig-Holstein and in the southern part of Germany, the concentrations of metolachlor-ESA and metolachlor-OXA are predicted to be particularly high in the north-east of the country. In contrast, metabolite CGA40172 shows a

Figure 93: Leachate concentrations for S-metolachlor and three metabolites

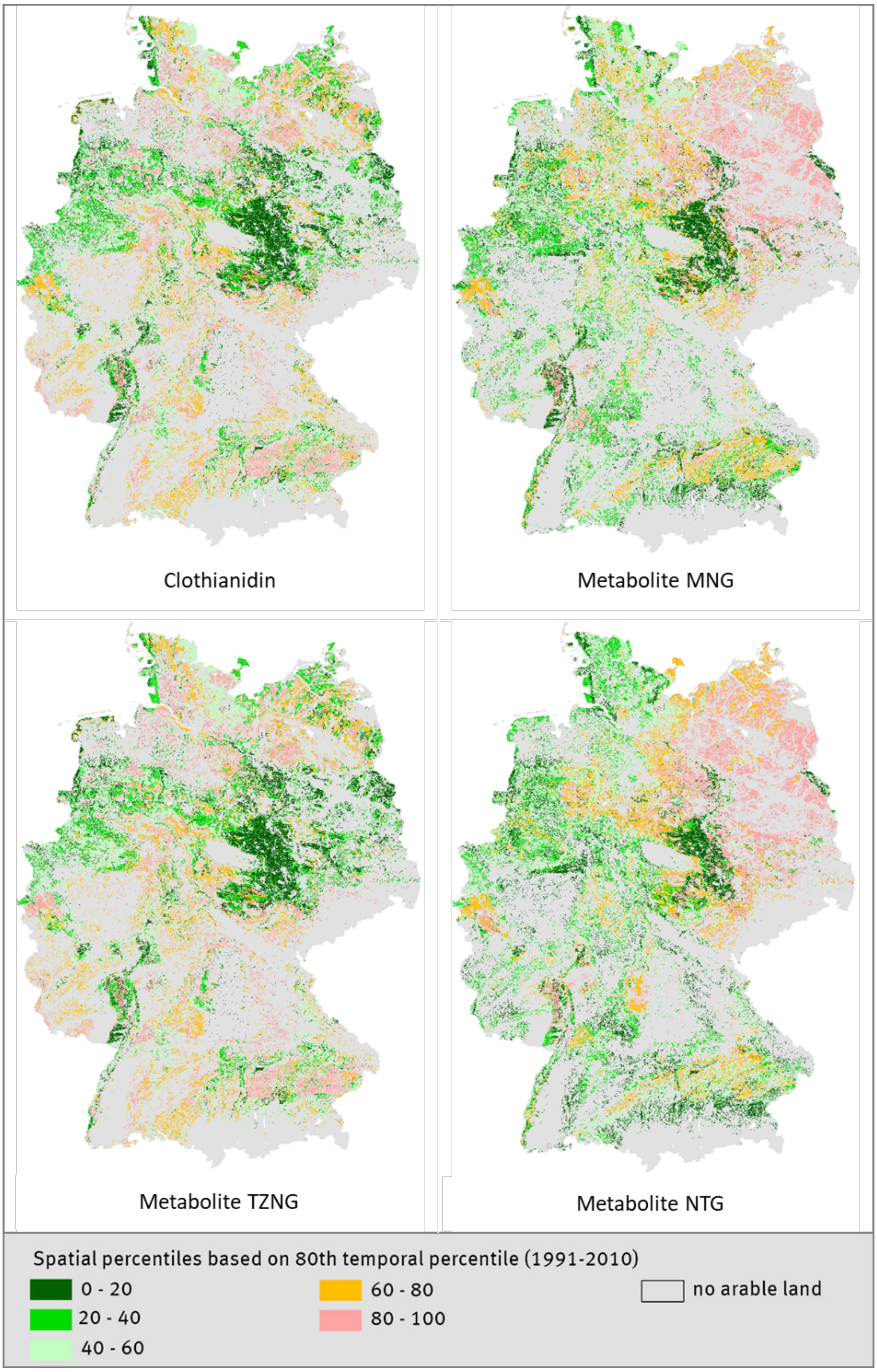
The annual leachate concentrations for S-metolachlor and its metabolites at 1 m soil depth are based on spring application in maize and calculated with the GeoPELMO DE version considering chromatographic and preferential flow, runoff and drainage (FOCUS L+R+M+D). The modelled concentrations are illustrated in five percentile classes.



Source: own illustration, Fraunhofer IME.

Figure 94: Leachate concentrations for clothianidin and three metabolites

The annual leachate concentrations for clothianidin and its metabolites at 1 m soil depth are based on spring application in sugar beets and calculated with the GeoPELMO DE version considering chromatographic and preferential flow, runoff and drainage (FOCUS L+R+M+D). The modelled concentrations are illustrated in five percentile classes.



Source: own illustration, Fraunhofer IME.

comparatively similar distribution of concentration as the active substance. The most reasonable explanation is that the sorption constant of metabolite CGA 40172 is quite similar to the parent compound S-metolachlor, whereas the metabolites ESA and OXA are hardly bound to the soil matrix.

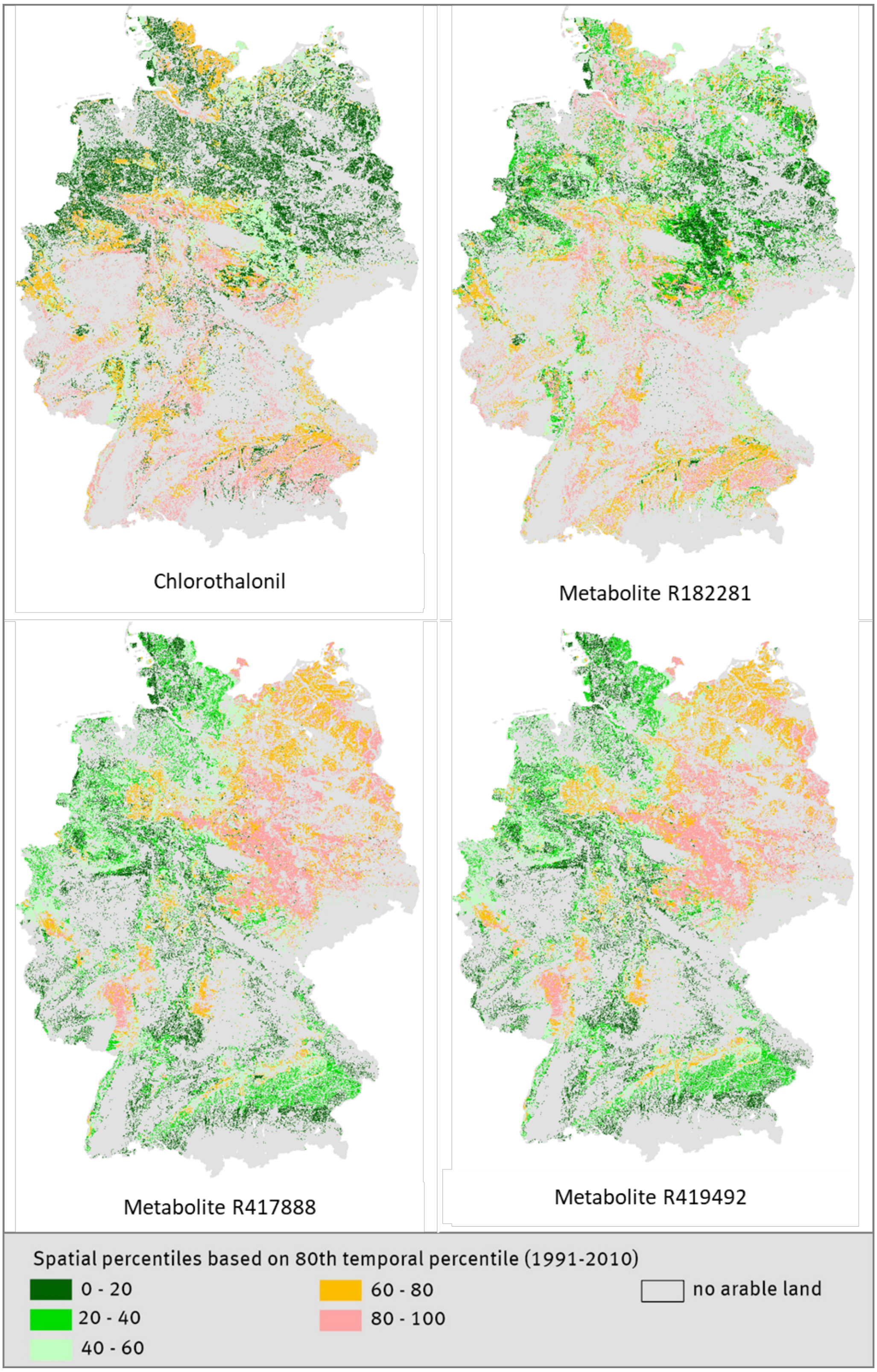
S-metolachlor can be considered as moderate substance regarding sorption and degradation. This is supported by a GUS-index of 2.3. In contrast, clothianidin has unfavourable properties for leaching, because the active substance is more persistent and more mobile. This is supported by a higher GUS value of 4.6 (see Figure 92). Hence, as indicated in Figure 94, a difference in the spatial distribution of percolate concentration compared to S-metolachlor (Figure 93) can be observed since larger areas in Northern Germany are represented by higher percentile classes. However, the differences are only minor compared to the results for some of the metabolites. Both active substances show in general higher concentrations in south and south-west Germany than in the north-east and north-west. The low percentile class (0-20th) for clothianidin (and its metabolites) in large parts of the black soil areas in the northern, eastern and southern Harz foreland is striking, while concentrations in the 20th-40th percentile class are predicted for S-metolachlor in those areas. When looking at the nationwide concentration pattern for the three metabolites of clothianidin, TZNG is well comparable to the active substance. An explanation could be that the sorption constant of the metabolite TZNG (K_{foc}: 266.8 L/kg) is rather comparable to the parent compound (K_{foc}: 124 L/kg) whereas the other two metabolites are more mobile (K_{foc} for MNG: 16.5 L/kg, K_{foc} for NTG: 16 L/kg). This is supported by higher GUS values for MNG (5.7) and NTG (5.5) compared to clothianidin (4.6) and TZNG (3.3). It seems that lower K_{foc} values lead to a general shift of higher percentiles from western to eastern Germany. This phenomenon also seems to be linked to the prediction of percolate concentrations for metabolites which are formed in PELMO only after a certain time in the soil profile.

Regarding the fate properties, clothianidin has the highest GUS-index (4.6) of the selected active substances considered in this analysis and therefore a high leaching potential. In contrast, chlorothalonil has the lowest GUS-index of 0.4. The map in Figure 95 shows indeed a different concentration pattern as the map for clothianidin in Figure 94. In general, lower percentiles are in Northern Germany whereas higher percentiles are located mostly in southern and western Germany. This is rather comparable to the pattern for S-metolachlor, an active substance with a moderate GUS-index of 2.3.

Referring to the transformation products of chlorothalonil, the two metabolites R417888 and R419492 show similar pattern of estimated relative concentrations with high percentiles in eastern Germany and lower percentiles in western and southern Germany, while they are different to the parent compound. The results for the third metabolite R182281 are different with generally lower concentrations in the north and higher concentrations in the south. That can only be explained by the properties of these metabolites since they are all formed as primary metabolites from the same parent compound. Major differences are again observed for the sorption constants for the three transformation products. Whereas metabolite R182281 has a rather high sorption value (K_{foc}: 386 L/kg), the two metabolites R417888 (K_{foc}: 9.5 L/kg) and R419492 (K_{foc}: 0.1 L/kg) show hardly any sorption to soil. Obviously, low sorption constants for metabolites lead to high estimated concentrations percentiles in the north-eastern part of Germany. Whether macropore flow is dominant or not doesn't seem of relevance for the estimation of percolate concentrations for the metabolites. This has been already concluded in earlier sections. However, if metabolites are sorbing more strongly to the soil, higher percolate volumes and the presence of macropore flow are probably key parameters for higher concentrations in the leachate. This would explain why higher concentrations of such compounds are often predicted in the southern regions of Germany.

Figure 95: Leachate concentrations for chlorothalonil and three metabolites

The annual leachate concentrations for chlorothalonil and its metabolites at 1 m soil depth are based on spring application in winter cereals and calculated with the GeoPELMO DE version considering chromatographic and preferential flow, runoff and drainage (FOCUS L+R+M+D). The modelled concentrations are illustrated in five percentile classes.



Source: own illustration, Fraunhofer IME.

The spatial distribution of estimated percolate concentrations for three active substances (S-metolachlor, clothianidin and chlorothalonil) and their main transformation products were discussed in this chapter in detail. When looking at the spatial pattern of the 80th temporal percentiles for these compounds presented it can be concluded that the known key parameters for FOCUS leaching modelling are still main drivers for the percolate concentrations, when additional processes are considered in spatial distributed modelling, e.g., similar sorption constants lead to similar spatial pattern even if active substances and transformation products are compared and the crop is different.

6.2.3 Protection level based on the FOCUS modelling approach

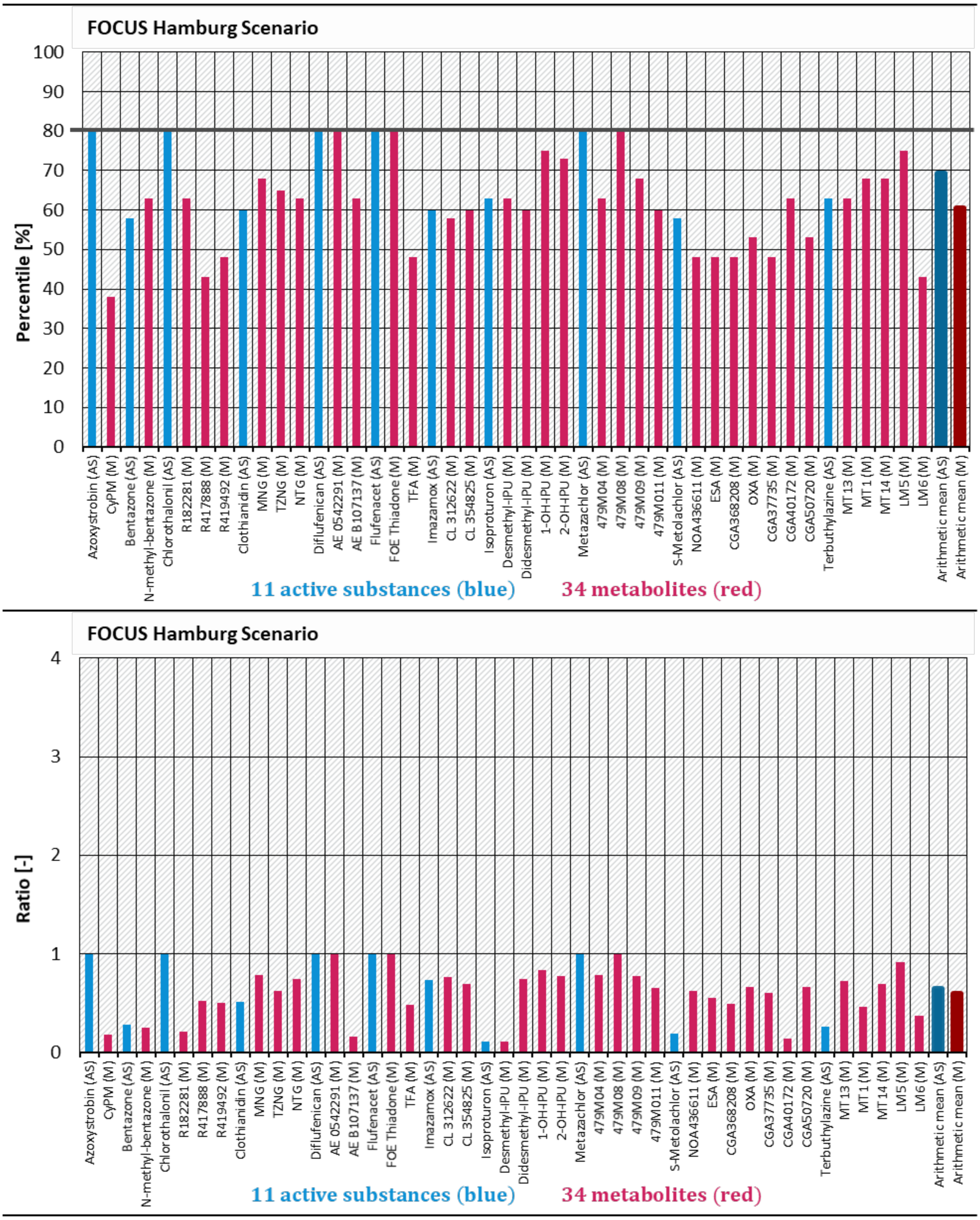
In this chapter the impact and possible consequences of the two proposed single scenarios on the national groundwater risk assessment are evaluated and discussed based on real pesticide uses. The two scenarios 6739/2804 Barsinghausen-Hohenbostel and 6126/2620/Hohwacht were previously selected based on maximum overlaps from modelling runs with fictive compounds, metabolites and application patterns and the GeoPELMO DE (FOCUS L) version considering the FOCUS modelling approach. The level of protection of the FOCUS Hamburg scenario and the two new scenarios is analysed for 11 active substances and 34 main transformation products. The predicted environmental concentrations (PECs) from the new scenarios are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (FOCUS L) for the agricultural area in Germany. The PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).

The results demonstrate that higher concentrations are systematically simulated with GeoPELMO DE (FOCUS L) for most of the selected active substances and metabolites compared to the FOCUS Hamburg scenario. This confirms the conclusion of the previous evaluation performed for fictive compounds in chapter 5.5. For five of 11 active substances and three of 34 metabolites the FOCUS Hamburg scenario reaches the 80th spatial percentile and a ratio of 1 compared to GeoPELMO DE (FOCUS L) (see Figure 97). This is mainly the case for compounds with PECs far below 0.1 µg/L. For all other compounds the 80th spatial percentile is not covered by the Hamburg scenario. For all active substances, the spatial percentiles of FOCUS Hamburg compared to GeoPELMO results (FOCUS L) for the agricultural area in Germany range between 58 % and 80 %, and an arithmetic mean percentile of 69 % is calculated. Those results are rather in line with the calculated protection level for dummy active substances (chapter 5.5.1). The ratios between the PECs from FOCUS Hamburg and GeoPELMO DE range between 0.11 and 1.0, and an arithmetic mean ratio of 0.64 is calculated.

For all metabolites, the spatial percentiles of FOCUS Hamburg compared to GeoPELMO DE (FOCUS L) results for the agricultural area in Germany range between 38 % and 80 %, and an arithmetic mean percentile of 61 % is calculated. The ratios between the PECs from FOCUS Hamburg and GeoPELMO DE range between 0.11 and 1.0, and an arithmetic mean ratio of 0.60 is calculated. This confirms that results from spatial distributed modelling with GeoPELMO DE are more conservative for a rather high portion of real active substances and metabolites, even when the FOCUS leaching approach is considered and all additional processes (macropore flow, runoff, drainage) are switched off. The FOCUS Hamburg scenario rather represents an averaged spatial 60th to 70th percentile than a realistic worst-case situation represented by an 80th spatial percentile.

Figure 96: Protection level of the FOCUS Hamburg scenario compared to GeoPELMO DE simulations for real active substances and their metabolites

Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the FOCUS Hamburg scenario are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

However, when comparing the alternative scenarios with GeoPELMO DE results, the concentrations simulated for 6739/2804/Barsinghausen-Hohenbostel and 6126/2620/Hohwacht seem to match better the 80th spatial percentile concentrations calculated with GeoPELMO DE (FOCUS L) for active substances and metabolites. These results are confirmed by the percentiles and ratios provided in Figure 97 and Figure 98.

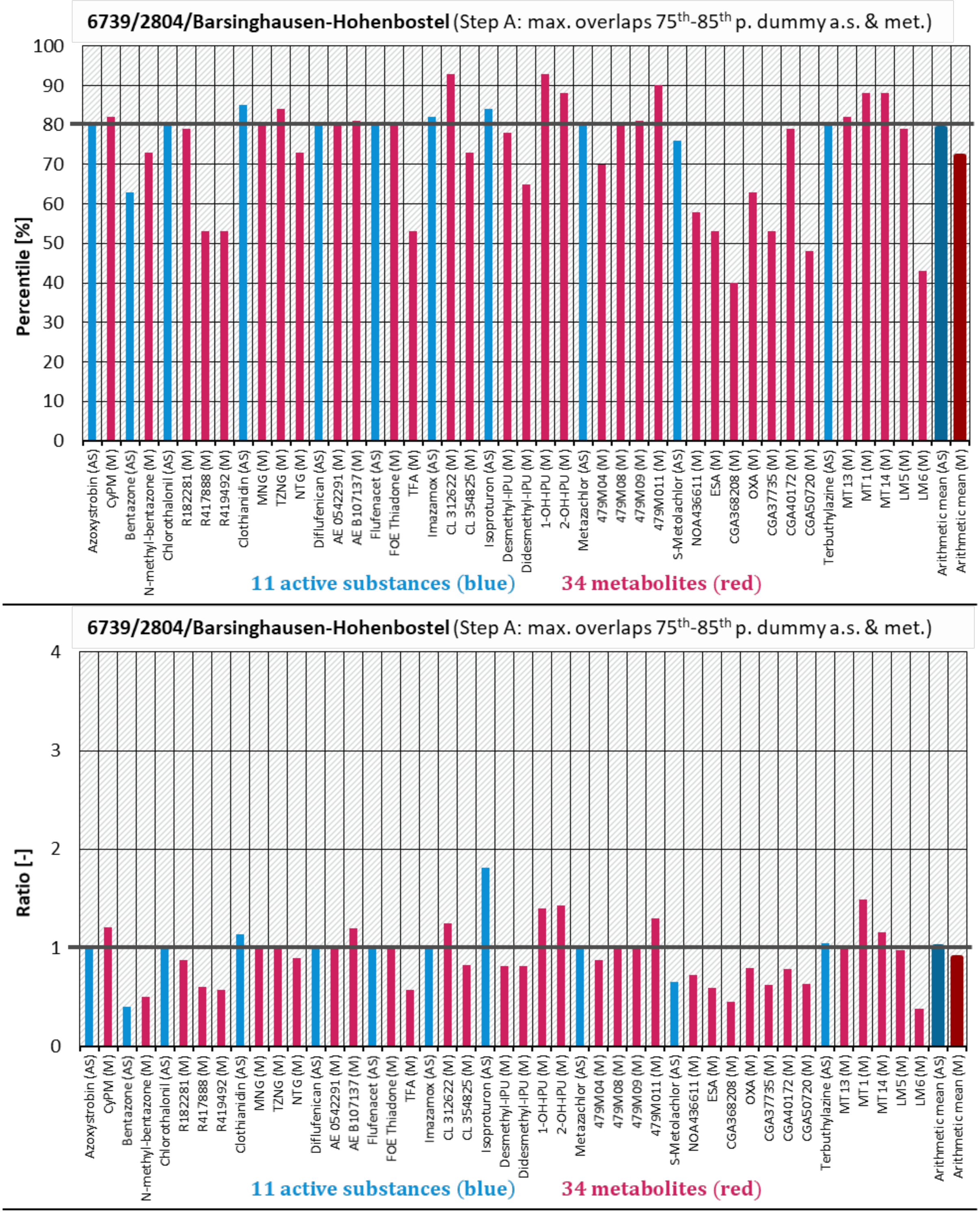
The PECs from most of the 11 active substances reach the 80th spatial percentile and a ratio of 1 or are above in both scenarios compared to GeoPELMO DE (FOCUS L). For all active substances, the spatial percentiles of 6739/2804/Barsinghausen-Hohenbostel compared to GeoPELMO DE (FOCUS L) results for the agricultural area in Germany range between 63 % and 85 %, and an arithmetic mean percentile of 79 % is calculated. The ratios between the PECs from Barsinghausen-Hohenbostel and GeoPELMO DE range between 0.40 and 1.81, and an arithmetic mean ratio of 1.01 is calculated. For all active substances, the spatial percentiles of 6126/2620/Hohwacht compared to GeoPELMO DE (FOCUS L) results for the agricultural area in Germany range between 73 % and 88 %, and an arithmetic mean percentile of 81 % is calculated. The ratios between the PECs from Hohwacht and GeoPELMO DE range between 0.89 and 1.41, and an arithmetic mean ratio of 1.08 is calculated. Those results confirm that PECs estimated for active substances with both scenarios are quite comparable to the targeted 80th spatial percentile in GeoPELMO DE (FOCUS L) and rather independent from compound properties.

The situation is slightly different for transformation products since more metabolites do not reach the 80th spatial percentile and a ratio of 1 in both scenarios compared to GeoPELMO DE (FOCUS L). For all metabolites, the spatial percentiles of 6739/2804/Barsinghausen-Hohenbostel compared to GeoPELMO DE (FOCUS L) results for the agricultural area in Germany range between 40 % and 93 %, and an arithmetic mean percentile of 72 % is calculated. The ratios between the PECs from Barsinghausen-Hohenbostel and GeoPELMO DE range between 0.38 and 1.49, and an arithmetic mean ratio of 0.91 is calculated. For all metabolites, the spatial percentiles of 6126/2620/Hohwacht compared to GeoPELMO DE (FOCUS L) results for the agricultural area in Germany range between 43 % and 93 %, and an arithmetic mean percentile of 71 % is calculated. The ratios between the PECs from Hohwacht and GeoPELMO DE range between 0.39 and 1.79, and an arithmetic mean ratio of 0.91 is calculated. Those results show that PECs estimated for metabolites with both scenarios represent a wider range compared to the targeted 80th spatial percentile in GeoPELMO DE (FOCUS L). However, similar average percentiles of 72 % and 71 % are calculated for 6739/2804/Barsinghausen-Hohenbostel and 6126/2620/Hohwacht based on 34 different transformation products. Besides, the range of ratios for both scenarios is not very different compared to active substance calculations. Taking all values into account, the results seem still acceptable since modelling of percolate concentrations for metabolites is generally connected to higher uncertainties.

It confirms that the soil-climate combinations 6739/2804/Hohenbostel and 6126/2620/Hohwacht are acceptable alternative scenarios for active substances and their transformation products, when the FOCUS leaching approach of chromatographic flow in the unsaturated soil zone is considered and additional processes like macropore flow, runoff and drainage are switched off. It should be taken into account that the range of ratios for transformation products formed by the same active substance can be huge (*e.g.,* Desmethyl-IPU and 1-OH-IPU) which means that it is difficult to find one scenario which is able to reach the exact 80th percentile concentrations from GeoPELMO DE for all transformation products of the metabolism scheme. This is a general conceptional point that should be considered in future when single scenarios are derived from spatial distributed leaching models.

Figure 97: **Protection level of the scenario Barsinghausen-Hohenbostel compared to GeoPELMO DE simulations for real active substances and their metabolites**

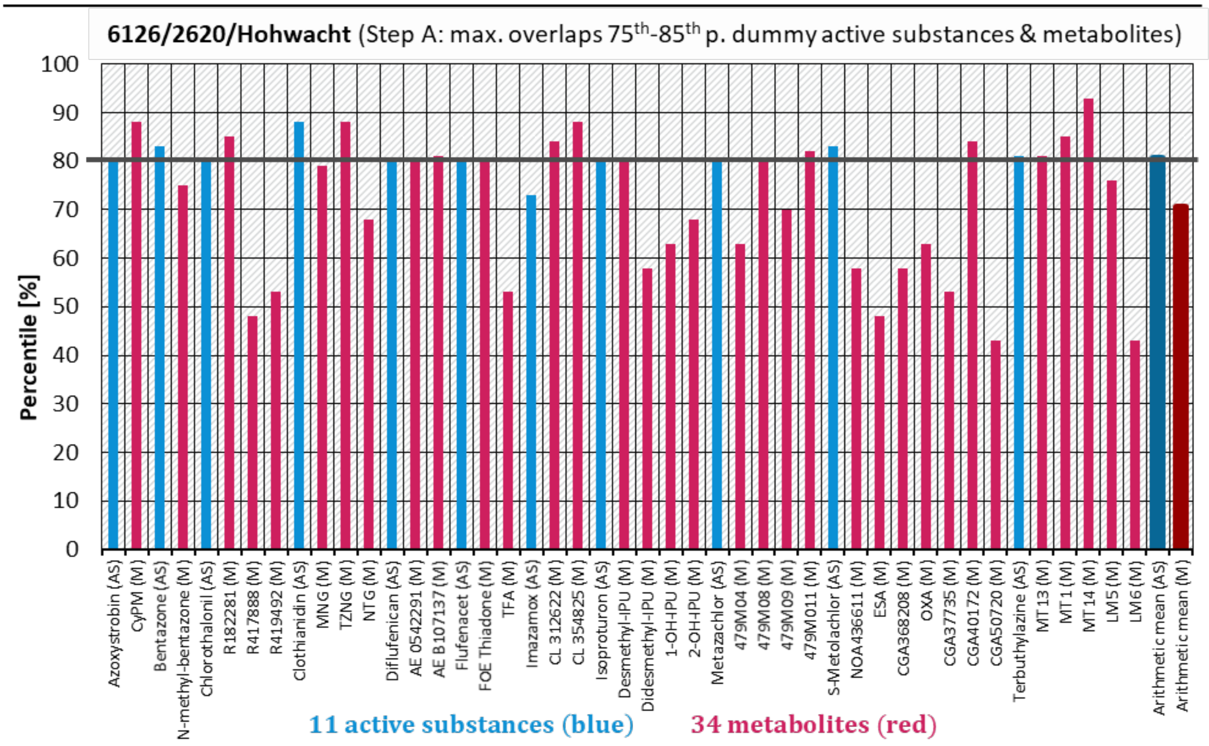
Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the new scenario Barsinghausen-Hohenbostel are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).

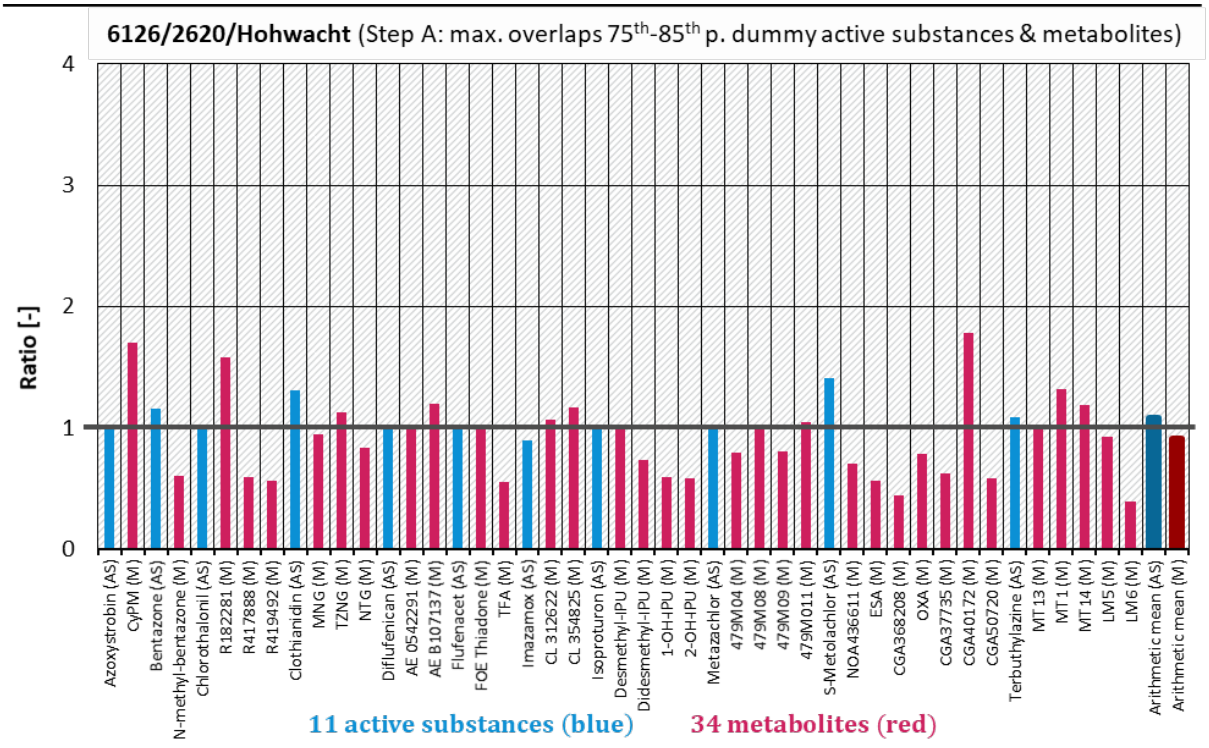


Source: own illustration, Fraunhofer IME.

Figure 98: Protection level of the scenario Hohwacht compared to GeoPELMO DE simulations for real active substances and their metabolites

Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the new scenario Hohwacht are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).





Source: own illustration, Fraunhofer IME.

6.2.4 Protection level considering chromatographic and preferential flow, runoff and drainage

In this chapter the impact and possible consequences of the six proposed single scenarios on the national groundwater risk assessment are evaluated and discussed based on real pesticide uses. The six scenarios 6135/2620/Hohwacht, 3162/798/Ulm, 7344/2352/Bad Harzburg, 935/379/Grambek, 9854/10464/Burgwald-Bottendorf and 1945/570/Schleswig were selected based on different overlapping strategies from modelling runs with fictive compounds, metabolites and application patterns and the GeoPELMO DE version considering chromatographic and preferential flow, runoff and drainage (version FOCUS L+R+M+D). The level of protection of the FOCUS Hamburg scenario and the six new scenarios is analysed for 11 active substances and 34 main transformation products. The predicted environmental concentrations (PECs) from the new scenarios are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE for the agricultural area in Germany. The PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).

The results demonstrate that higher concentrations are systematically simulated with GeoPELMO DE (FOCUS L+R+M+D) for almost all active substances and metabolites compared to the FOCUS Hamburg scenario. This is not surprising as it confirms the conclusion of the previous evaluation for fictive compounds in chapter 5.5 that FOCUS Hamburg does not represent the 80th spatial percentile of annual concentrations in the percolate at 1 m depth. For all active substances except one and for all metabolites the FOCUS Hamburg scenario does not reach the 80th spatial percentile and a ratio of 1 compared to GeoPELMO DE (FOCUS L+R+M+D) (see Figure 99). Apart from chlorothalonil, clothianidin and imaxamox FOCUS Hamburg represent percentiles below 50 %. However, for chlorothalonil only percolate concentrations below 0.001 µg/L have been simulated. For clothianidin the PECs were simulated based on incorporated seed treatment that means that macropore flow will become less dominant.

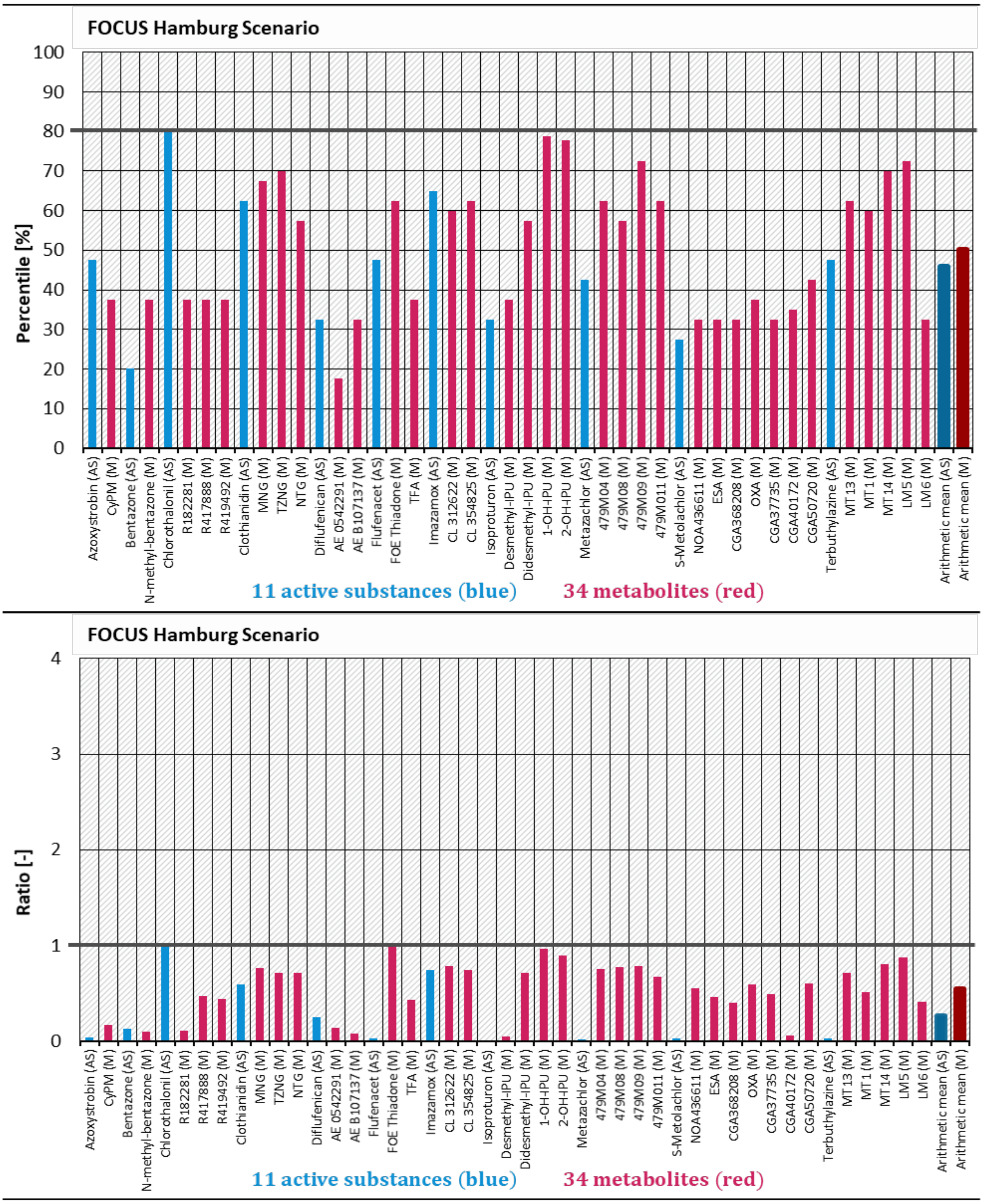
For all active substances, the spatial percentiles of FOCUS Hamburg compared to GeoPELMO DE (FOCUS L+R+M+D) results for the agricultural area in Germany range between 20 % and 80 %, and an arithmetic mean percentile of 46 % is calculated. Those results are in line with the calculated protection level for dummy active substances, where the PECs from the FOCUS Hamburg scenario represented a range from the 25th to the 66th percentile of nationwide distributed PECs and the arithmetic mean of the percentiles was also 46 % (chapter 5.5.1). The ratios between the PECs from FOCUS Hamburg and GeoPELMO DE range between 0.01 and 1.0, and an arithmetic mean ratio of 0.26 is calculated.

For all metabolites, the spatial percentiles of FOCUS Hamburg compared to GeoPELMO DE (FOCUS L+R+M+D) results for the agricultural area in Germany range between 18 % and 79 %, and an arithmetic mean percentile of 50 % is calculated. Those results deviate from the calculated protection level for dummy metabolites, where the PECs from the FOCUS Hamburg scenario represented a smaller and higher range between the 53th and the 80th percentile of nationwide distributed PECs, and an arithmetic mean of 67 % was calculated (chapter 5.5.2). The ratios between the PECs from FOCUS Hamburg and GeoPELMO DE show also a large range between 0.05 and 1.0, and an arithmetic mean ratio of 0.55 is calculated.

This confirms that results from spatial distributed modelling with GeoPELMO DE (version FOCUS L+R+M+D) are more conservative for almost all tested real active substances and their main metabolites, when the FOCUS leaching approach is completed with additional processes like macropore flow, runoff and drainage. The FOCUS Hamburg scenario rather represents only a medium spatial percentile for both active substances and metabolites than a realistic worst-case situation represented by an 80th spatial percentile.

Figure 99: **Protection level of the FOCUS Hamburg scenario compared to GeoPELMO DE simulations for real active substances and their metabolites**

Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the FOCUS Hamburg scenario are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L+R+M+D) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

When comparing the alternative scenarios with GeoPELMO DE (FOCUS L+R+M+D), the concentrations simulated for 6135/2620/Hohwacht, 3162/798/Ulm and 7344/2352/Bad Harzburg seem to match the 80th spatial percentile concentrations obtained with GeoPELMO DE well for active substances. The percentiles calculated for the three alternative locations are rather close to the aimed 80th percentile. This observation is consistent with the scenario selection method for step B (6135/2620/Hohwacht and 3162/798/Ulm) and step C (7344/2352/Bad Harzburg), which both represent the maximum overlap for active substances. In contrast, results for 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig seem to be more heterogeneous and less protective like the FOCUS Hamburg scenario.

For example, for all active substances, the spatial percentiles of 6135/2620/Hohwacht compared to GeoPELMO DE (FOCUS L+R+M+D) results for the agricultural area in Germany range between 73 % and 93 %, and an arithmetic mean percentile of 76 % is calculated. The ratios between the PECs from the scenario and GeoPELMO DE range between 0.72 and 1.43, and an arithmetic mean ratio of 0.89 is calculated (see Figure 100). The spatial percentiles of 3162/798/Ulm compared to GeoPELMO DE (FOCUS L+R+M+D) results range between 63 % and 93 %, and an arithmetic mean percentile of 73 % is calculated. The ratios between the PECs from the scenario and GeoPELMO DE range between 0.32 and 1.59, and an arithmetic mean ratio of 0.84 is calculated (see Figure 101). The spatial percentiles of 7344/2352/Bad Harzburg compared to GeoPELMO DE (FOCUS L+R+M+D) results range between 43 % and 98 %, and an arithmetic mean percentile of 84 % is calculated. The ratios between the PECs from the scenario and GeoPELMO DE range between 0.51 and 2.84, and an arithmetic mean ratio of 1.59 is calculated (see Figure 102).

The three scenarios 6135/2620/Hohwacht, 3162/798/Ulm and 7344/2352/Bad Harzburg represent soil-climate-combinations where macropore flow is included, whereas sandy soils occur at the other three locations 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig, and only chromatographic flow is considered. This provides some evidence at least for active substances that to give some certainty that a selected scenario covers the 80th spatial percentile calculated with GeoPELMO DE, soil profiles representing macropore flow class 2 or 3 should be selected.

To provide a comparison, lower average spatial percentiles (arithmetic mean) for active substances of 41 %, 53 % and 42 % and lower average ratios (arithmetic mean) of 0.29, 0.50 and 0.32 were calculated for 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig compared to GeoPELMO DE (FOCUS L+R+M+D) results, respectively. This observation can be explained with the scenario selection method for step D for 69854/10464/Burgwald-Bottendorf and step L for 1945/570/Schleswig, which both represent a maximum overlapping for metabolites. The scenario selection method for step E for 935/379/Grambek represents a maximum overlapping for dummy active substances and spring application. Therefore, the low spatial percentile for real active substances is rather surprising.

In contrast to active substances, the protection goal and pattern for transformation products is rather complicated and more heterogeneous regarding cover a realistic worst-case situation (80th percentile) from spatially distributed percolate concentrations. Nevertheless, the PECs simulated for 6135/2620/Hohwacht and 3162/798/Ulm (both scenarios are selected based on maximum overlapping for both active substances and metabolites) seem to cover the concentrations obtained with GeoPELMO DE (FOCUS L+R+M+D) better than the other four scenarios. The results for 7344/2352/Bad Harzburg, 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig are less protective for several metabolite situations.

These results are confirmed by the percentile calculation. On average, the best performance compared to GeoPELMO DE (FOCUS L+R+M+D) was found for Ulm and with some limitations for Hohwacht as indicated by the high arithmetic mean percentiles close to 80 %. For example, for all metabolites, the spatial percentiles of 6135/2620/Hohwacht compared to GeoPELMO DE (FOCUS L+R+M+D) results for the agricultural area in Germany range between 43 % and 93 %, and an arithmetic mean percentile of 70 % is calculated. The ratios between the PECs from the scenario and GeoPELMO DE range between 0.43 and 1.59, and an arithmetic mean ratio of 0.84 is calculated (see Figure 100). The spatial percentiles of 3162/798/Ulm compared to GeoPELMO DE (FOCUS L+R+M+D) results range between 53 % and 93 %, and an arithmetic mean percentile of 74 % is calculated. The ratios between the PECs from the scenario and GeoPELMO DE range between 0.37 and 1.41, and an arithmetic mean ratio of 0.86 is calculated (see Figure 101).

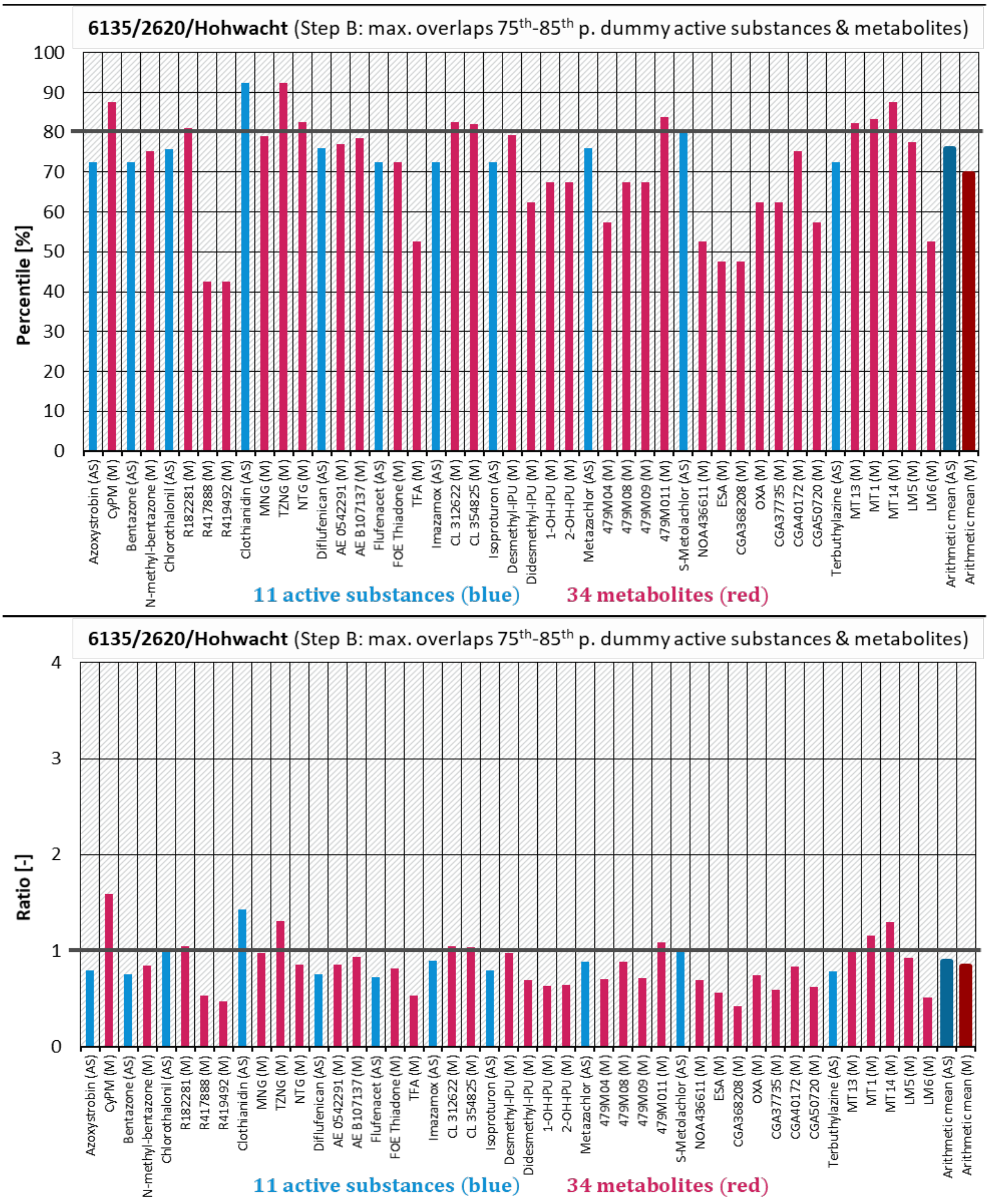
To provide a comparison, lower average spatial percentiles (arithmetic mean) for metabolites of 52 %, 60 %, 65 % and 48 % were calculated for 7344/2352/Bad Harzburg, 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig compared to GeoPELMO DE (FOCUS L+R+M+D) results, respectively. (see Figure 102, Figure 103, Figure 104, Figure 105). Lower average ratios (arithmetic mean) of 0.79, 0.65, and 0.57 were calculated for Bad Harzburg, Burgwald-Bottendorf and Schleswig, while a higher average ratio (arithmetic mean) of 1.05 was calculated for Grambek. The average ratio of 1.05 for scenario Grambek is accompanied by a large range of ratios between 0.003 and 3.25. It can be observed from the percentile and ratio analysis that both scenarios 69854/10464/Burgwald-Bottendorf (selection step D) and 1945/570/Schleswig (selection step L), which both represent a maximum overlapping for dummy metabolites do not represent a balanced result for all analysed real metabolites.

The calculated values show in particular that there can be still a large range of percentiles and ratios represented for metabolites originated from the same active compound (*e.g.,* parent compound chlorothalonil: 76 %, metabolite R182281: 81 %, metabolite R417888: 43 %, metabolite R419492: 43 % in Hohwacht or parent compound chlorothalonil: 88 %, metabolite R182281: 88 %, metabolite R417888: 28 %, metabolite R419492: 28 % in Bad Harzburg). It was previously concluded for active substances that only alternative scenarios which are represented by macropore flow class 2 or 3 lead to similar results as the 80th spatial percentile from GeoPELMO DE simulations. The situation seems to be different for transformation products because the concentrations were, for example, often underestimated by the macropore scenario 7344/2352/Bad Harzburg. On average, higher concentrations were simulated for the soil-climate-combination 935/379/Grambek representing macropore class 1 (no macropores). Obviously, macropore flow doesn't play such a dominant role for transformation products compared to active substances.

Finally, the best performance for metabolites can be expected from the scenarios 6135/2620/Hohwacht and 3162/798/Ulm and with some limitation from 935/379/Grambek. For 935/379/Grambek (no macropore flow) higher concentrations are simulated than for 7344/2352/Bad Harzburg (with macropore flow). The range of ratios (PECs from single scenario compared to 80th spatial percentile in GeoPELMO DE (FOCUS L+R+M+D)) for transformation products formed by the same active substance can be huge in the same soil-climate-combination which means that it is difficult to find a scenario which is able to match 80th percentile concentrations from spatially distributed leaching modelling for all transformation products of one metabolism scheme.

Figure 100: Protection level of the scenario Hohwacht compared to GeoPELMO DE simulations for real active substances and their metabolites

Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the new scenario Hohwacht are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L+R+M+D) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).

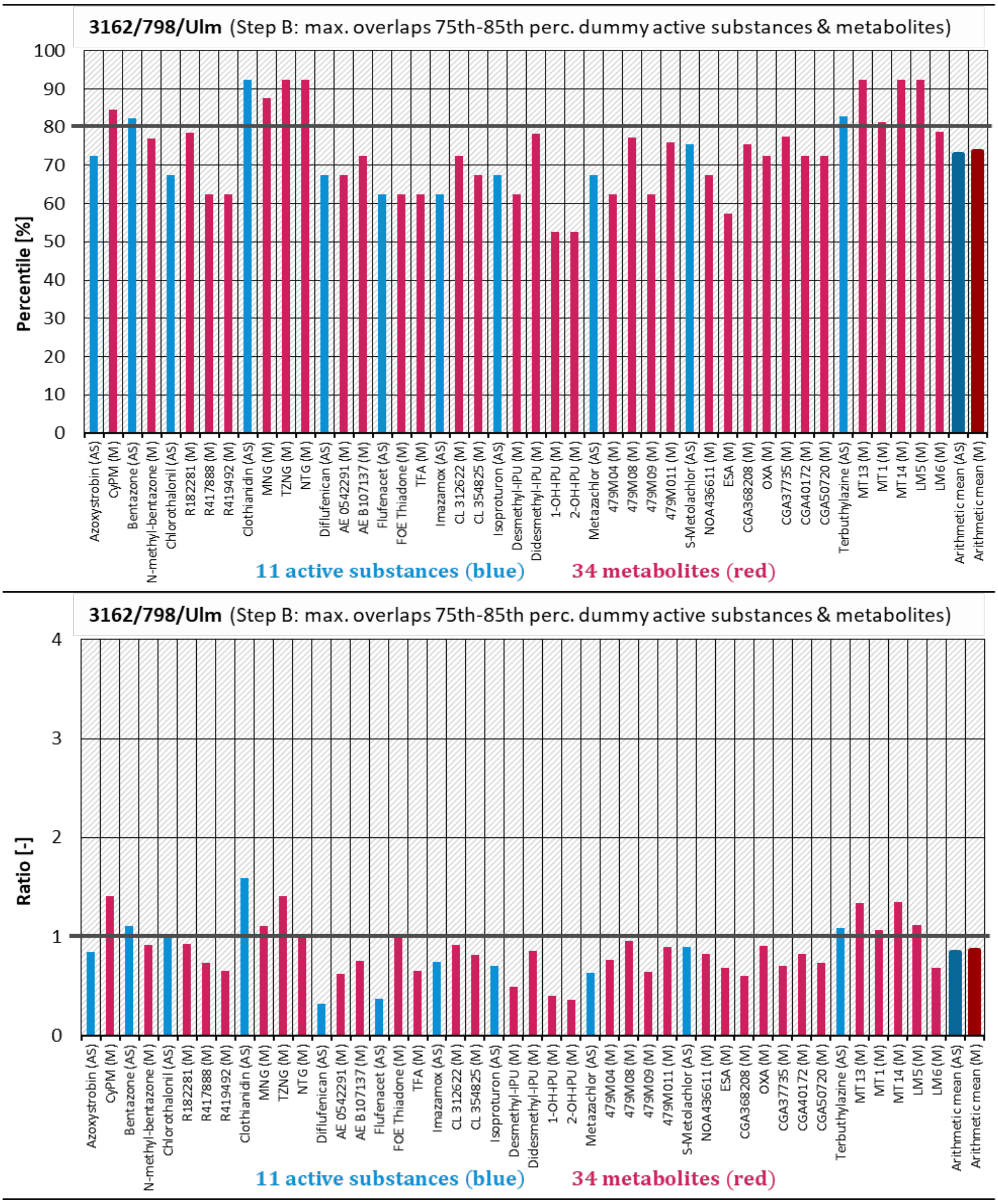


Source: own illustration, Fraunhofer IME.

Though the evaluation in this chapter is based on scenarios which were selected based on the results of dummy pesticide uses, more scenarios have been analysed with regard to their ability to represent the 80th percentile of GeoPELMO DE (FOCUS L+R+M+D) (see appendix C)

Figure 101: Protection level of the scenario Ulm compared to GeoPELMO DE simulations for real active substances and their metabolites

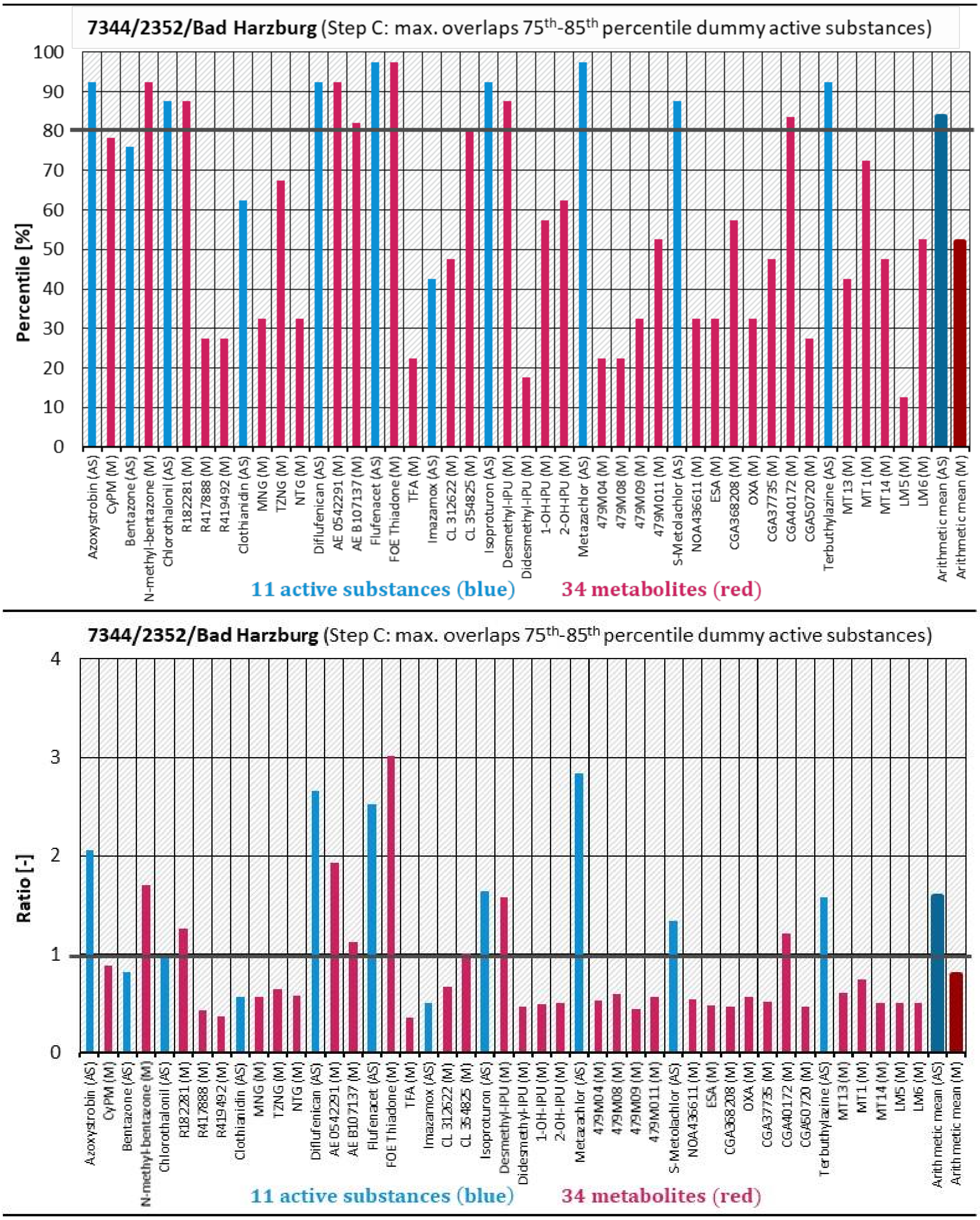
Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the new scenario Ulm are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L+R+M+D) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

Figure 102: **Protection level of the scenario Bad Harzburg compared to GeoPELMO DE simulations for real active substances and their metabolites**

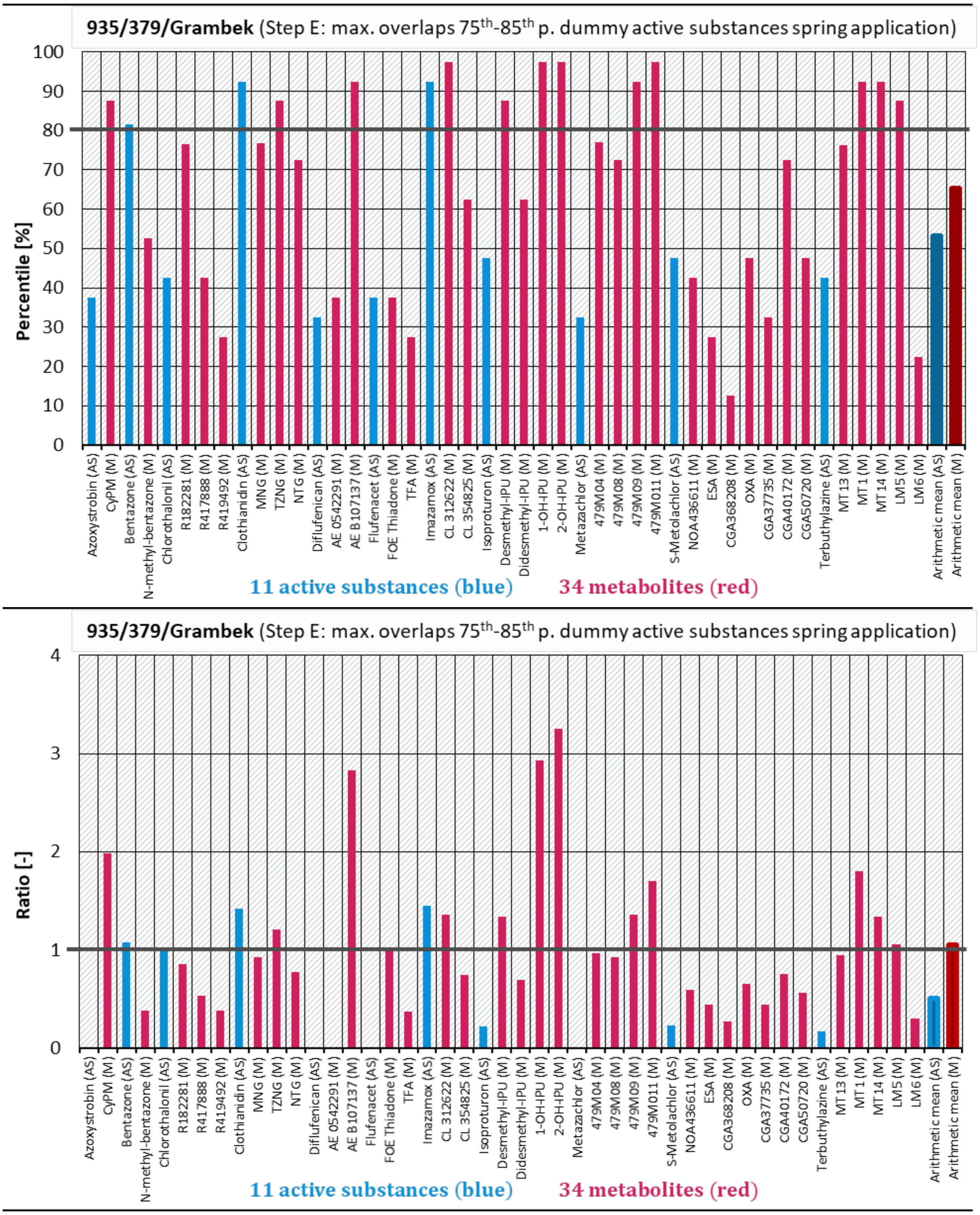
Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the new scenario Bad Harzburg are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L+R+M+D) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

Figure 103: Protection level of the scenario Grambek compared to GeoPELMO DE simulations for real active substances and their metabolites

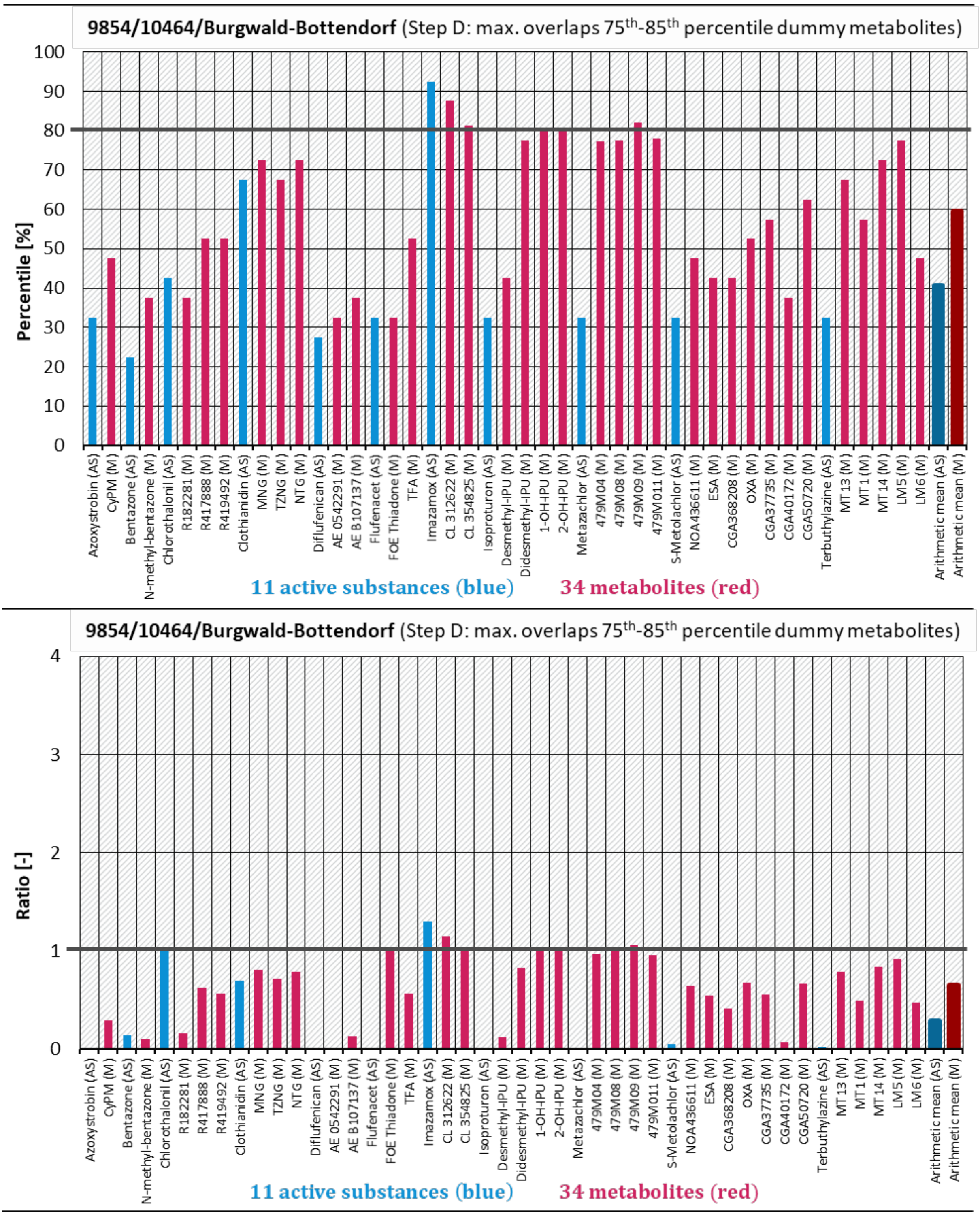
Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the new scenario Grambek are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L+R+M+D) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

Figure 104: **Protection level of the scenario Burgwald-Bottendorf compared to GeoPELMO DE simulations for real active substances and their metabolites**

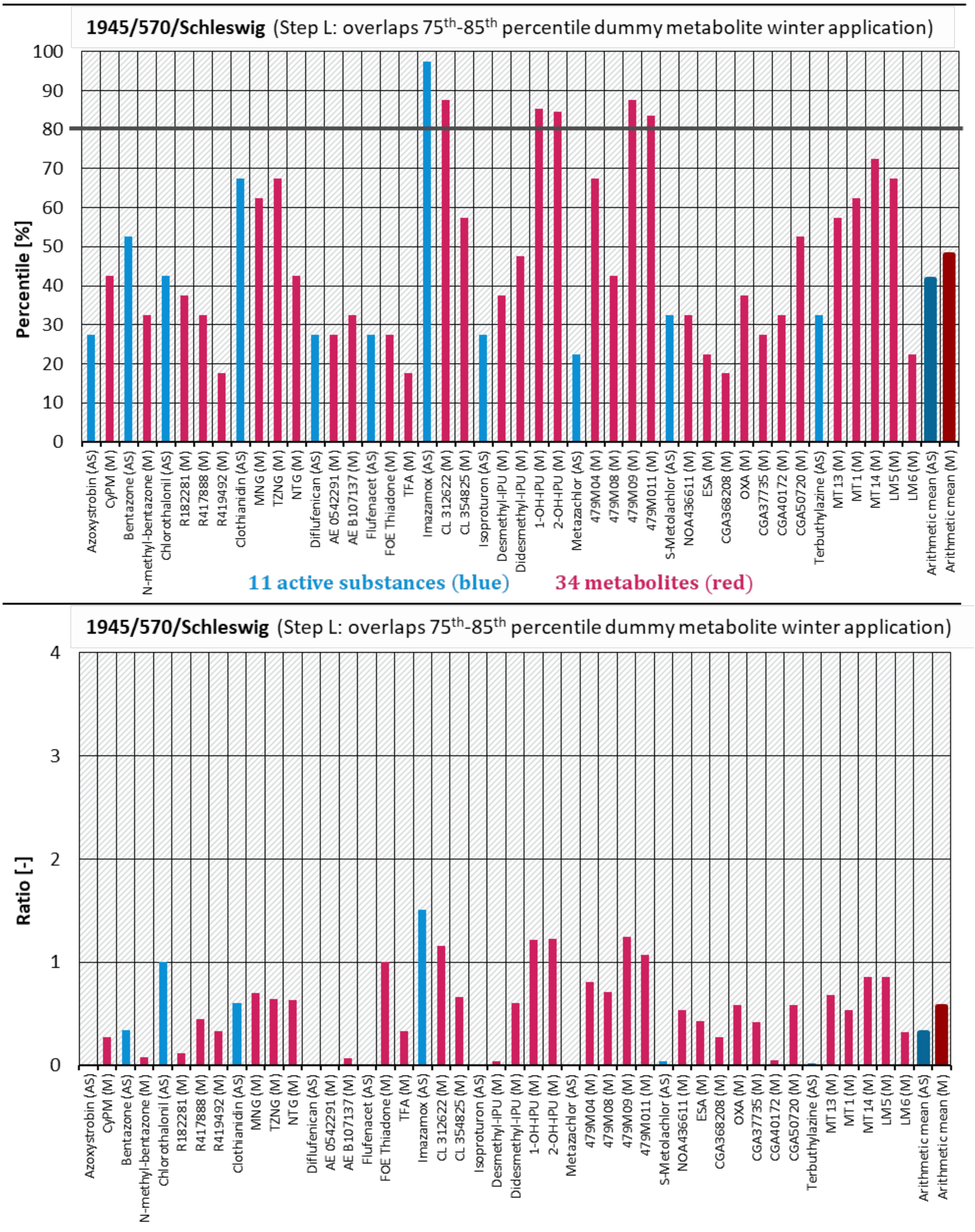
Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the new scenario Burgwald-Bottendorf are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L+R+M+D) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

Figure 105: Protection level of the scenario Schleswig compared to GeoPELMO DE simulations for real active substances and their metabolites

Model simulations are conducted for pesticide uses for 11 active substances and their main metabolites. The predicted environmental concentrations (PECs) from the new scenario Schleswig are compared as percentiles and ratios with the 80th spatial percentile from GeoPELMO DE (version FOCUS L+R+M+D) for the agricultural area in Germany. PECs are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

6.3 Summary and conclusion on scenario selection and protection level

In the following, a summary and conclusion regarding the selection of new scenarios from GeoPELMO DE (chapter 6.1) as well as the level of protection of the FOCUS Hamburg scenario (chapter 5.5) and alternative national scenarios (chapter 6.2) is provided.

Compared to the model FOCUS PELMO, which considers chromatographic flow in the unsaturated soil zone and is currently in use for regulatory decision making, the new spatial leaching model GeoPELMO DE includes additional processes like runoff, preferential flow (macropore flow) and drainage. Especially preferential flow is dominant for PEC calculation in large agricultural areas in Germany. This process leads to significant higher concentrations for spray applications than predicted with the Hamburg scenario in FOCUS PELMO. Incorporation of pesticide uses in soil (e.g. for seed treatments) reduces the influence of this process in PELMO. Furthermore, the influence of preferential flow on percolate concentrations for transformation products is rather limited. Compared to preferential flow, runoff and drainage have a lower influence on estimated percolate concentrations at 1 m soil depth.

Based on calculations for few fictive and more real pesticide uses, the FOCUS Hamburg scenario is not covering the 80th spatial percentile of two different GeoPELMO DE versions (FOCUS L and FOCUS L+R+M+D) in most situations. Higher percolate concentrations (80th spatial percentile) are simulated with GeoPELMO DE for most of the active substances and metabolites compared to the FOCUS Hamburg scenario.

A comparison with the model version which uses the FOCUS leaching approach of chromatographic flow only (FOCUS L) provides evidence that the percolate concentrations from FOCUS Hamburg represent a range between 52 % and 70 % for six dummy active substance situations (arithmetic mean: 61 %) and between 58 % and 80 % for 11 real active substances (arithmetic mean: 69 %) as well as between 38 % and 80 % for 34 real metabolites (arithmetic mean: 61 %). That means compared to the GeoPELMO DE version FOCUS L the spatial percentile for FOCUS Hamburg leachate concentrations is still below 80 % for a high number of evaluated compounds. On average values, the ratio between FOCUS Hamburg and GeoPELMO DE (FOCUS L) was found to be 0.64 for 11 real active substances (range: 0.11 to 1.0) and 0.60 for 34 real metabolites (range: 0.11 to 1.0).

A comparison with the model version which considers chromatographic and preferential flow, runoff and drainage (FOCUS L+R+M+D) confirms that percolate concentrations from FOCUS Hamburg represent a wider range between 25 % and 66 % (arithmetic mean: 46 %) for six dummy active substance situations, between 20 % and 80 % for 11 real active substances (arithmetic mean: 46 %), as well as between 53 % and 80 % for eight dummy metabolite situations (arithmetic mean: 67 %) and between 18 % and 79 % for 34 real metabolites (arithmetic mean: 50 %). Compared to the GeoPELMO DE version FOCUS L+R+M+D, the PECs from FOCUS Hamburg are rather representing a central situation for the agricultural area in Germany. The arithmetic mean percentiles for real 34 transformation products were lower compared to eight dummy metabolite situations presumably because secondary, tertiary and quaternary metabolites were considered, too. On average values, the ratio between FOCUS Hamburg and GeoPELMO DE (FOCUS L+R+M+D) concentrations was found to be 0.26 for 11 real active substances (range: 0.01 to 1.0) and 0.55 for 34 real metabolites (range: 0.05 to 1.0).

It can be finally concluded that the results from spatially distributed leaching modelling with GeoPELMO DE are more conservative as the current lower tier national groundwater risk assessment approach for a rather high portion of active substances and their metabolites. This finding is independent of whether the FOCUS leaching approach with chromatographic flow or an extended approach with additional processes such as preferential (macropore) flow, runoff and drainage is considered. However, the protection goal of the FOCUS Hamburg scenario is lower, when the leaching modelling approach is completed with preferential flow, runoff and drainage.

Considering the results of a rather low level of protection of the FOCUS Hamburg scenario compared to GeoPELMO DE, alternative scenarios were selected from the new PELMO model versions which better represent the 80th spatial percentile of national climate-soil conditions. This is principally confirming the outcome of the previous research project according to spatial distributed leaching modelling when different soil data with smaller scale have been used (Klein et al. 2019b). Alternative scenarios were selected in 11 different steps from two model versions of GeoPELMO DE, considering the FOCUS leaching approach with chromatographic flow (model version FOCUS L, step A) and considering chromatographic and preferential flow, runoff and drainage (model version FOCUS L+R+M+D, steps B-L). The main principle behind was to identify climate-soil combinations in GeoPELMO DE based on the highest possible number of overlaps of 14 percolate concentration maps from three dummy active substances and four metabolites in two crops in the range between the 75th and 85th spatial percentile.

Two national scenarios 6739/2804/Barsinghausen-Hohenbostel and 6126/2620/Hohwacht were identified from the GeoPELMO DE model version considering the FOCUS leaching approach (FOCUS L) which better cover the 80th spatial percentile of the agricultural area in Germany. Both climate-soil combinations represent rather small agricultural areas of 2 km² and 24 km². Both scenarios meet the 80 ± 5th spatial percentile for most of the dummy active substances and dummy transformation products. In few situations the estimated leaching concentrations represent a percentile above the 85th or below the 75th percentile. When comparing the two alternative scenarios with GeoPELMO DE (FOCUS L) for active substances from real pesticide uses, the concentrations simulated for 6739/2804/Barsinghausen-Hohenbostel and 6126/2620/Hohwacht are quite comparable to the targeted 80th spatial percentile in GeoPELMO DE (FOCUS L) and rather independent from compound properties. For 6739/2804/Barsinghausen-Hohenbostel, they range between 63 % and 85 %, and an arithmetic mean percentile of 79 % was calculated. For 6126/2620/Hohwacht, they range between 73 % and 88 %, and an arithmetic mean percentile of 81 % was calculated. For transformation products, the situation is slightly different. The metabolite concentrations simulated for 6739/2804/Barsinghausen-Hohenbostel range between 40 % and 93 %, and an arithmetic mean percentile of 72 % was calculated. The metabolite concentrations simulated for 6126/2620/Hohwacht are in a similar range between 43 % and 93 %, and an arithmetic mean percentile of 71 % was calculated. It shows that the protection level is not covered for all real tested metabolite situations with both scenarios. However, the calculating percolate concentrations for metabolites is generally connected to higher uncertainties. Therefore, the results for both scenarios seem to be still acceptable also for transformation products.

Based on the evaluations in the project, both 6739/2804/Barsinghausen-Hohenbostel and 6126/2620/Hohwacht can be finally recommended as suitable alternative scenarios for active substances and metabolites in comparison with the 80th spatial percentile from GeoPELMO DE (FOCUS L+R+M+D) when the FOCUS leaching concept of chromatographic flow is extended to the agricultural area in Germany.

Six scenarios 6135/2620/Hohwacht, 3162/798/Ulm, 7344/2352/Bad Harzburg, 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig were selected from the GeoPELMO DE versions considering chromatographic and preferential flow, runoff and drainage (FOCUS L-R+M+D) and are recommended as alternative national scenarios. They have been identified from a different number (13, 11, 6, 8, 3 and 4) of overlaps from 14 dummy percolate concentration maps and represent agricultural areas between 7 km² and 456 km². Two scenarios contain soils without macropore flow (9854/10464/Burgwald-Bottendorf, 935/379/Grambek), three scenarios represent soils with moderate macropore flow

(6135/2620/Hohwacht, 3162/798/Ulm, 1945/570/Schleswig) and one scenario contains a soil with high potential for macropore flow (7344/2352/Bad Harzburg). How much they finally cover the 80 ± 5th spatial percentile for all dummy active substances and dummy transformation products depends on the number of overlaps from the selection step. If the number of overlaps in this percentile range was low when the scenarios were selected, then the PEC deviations from this target protection level are more frequent and larger. The deviations can be characterised by higher and lower concentrations compared to percolate estimations from the 80th spatial percentile in GeoPELMO DE (FOCUS L-R+M+D).

When comparing the alternative scenarios with GeoPELMO DE (FOCUS L+R+M+D) for active substances from real pesticide uses, the concentrations simulated for 6135/2620/Hohwacht, 3162/798/Ulm and 7344/2352/Bad Harzburg were found to suitable represent the 80th spatial percentile concentrations obtained with GeoPELMO DE. In contrast, results for 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig seem to be more heterogeneous and less protective for parent compound. For transformation products, the situation is more heterogeneous. Nevertheless, the scenarios 3162/798/Ulm and 6135/2620/Hohwacht still represent the 80th spatial percentile of GeoPELMO DE quite acceptable. The results for 7344/2352/Bad Harzburg, 9854/10464/Burgwald-Bottendorf, 935/379/Grambek and 1945/570/Schleswig are less protective for several real metabolite situations. Especially the percentile and ratio analysis showed that both scenarios 69854/10464/Burgwald-Bottendorf and 1945/570/Schleswig, which both represent a maximum overlapping for dummy metabolites do finally not represent balanced percolate concentrations for all analysed real metabolites.

Based on the evaluations in the project, both 6135/2620/Hohwacht and 3162/798/Ulm and with limitations 7344/2352/Bad Harzburg are recommended as most suitable alternative scenarios which lead to most stable modelling results for active substances and metabolites in comparison with the 80th spatial percentile from GeoPELMO DE (FOCUS L+R+M+D) considering all additional processes for leaching. The results provide further evidence that there is no guarantee that a specific protection level is covered by those three single scenarios and other climate-soil-combinations for all possible pesticide uses in the regulatory framework.

Independent on the selected scenario a large range of percentiles and ratios was repeatedly found for the active substance and subsequent transformation products of one metabolism scheme. This means that a single scenario can hardly be used to guarantee a realistic worst-case situation for all compounds of a given metabolism scheme. The analysis showed that the spatial 80th percentile concentration in a model like GeoPELMO DE would always be represented by different individual climate-soil-combinations for the compounds of one degradation scheme. This result was found to be independent from the model version of GeoPELMO DE. However, the modelling results are more heterogeneous and complex when additional processes like runoff, preferential flow and drainage are considered to estimate percolate concentrations in the unsaturated soil zone.

Considering the overall results of the analysis performed in this project, the following conclusions can be drawn for regulatory decision making. To reach the GeoPELMO DE (FOCUS L) results on an average, an uncertainty factor of two could be considered for active substances and metabolites when simulations are performed with the standard FOCUS Hamburg scenario. This factor would not include the influence of macropore flow, run-off and drainage for estimating percolate concentrations. To reach the GeoPELMO DE (FOCUS L+R+M+D) result on average, an uncertainty factor of three for active substances and a factor of two for metabolites could be considered when simulations are performed with the FOCUS Hamburg scenario. This factor would include the influence of macropore flow, run-off and drainage. To cover all tested pesticide situations an assessment factor of 10 would be required to correct the FOCUS

Hamburg result in terms of GeoPELMO DE (FOCUS L+R+M+D) results. From a modelling perspective, it can be concluded that finally only a spatial model such as GeoPELMO DE would be able to calculate an exact temporal and spatial 80th percentile for all active substances and metabolites independent on their properties, their position in the metabolism scheme and independent from the pesticide application pattern. However, the calculation time of such a high-resolution model as GeoPELMO must be considered. The use of a single scenario can be used as an approximation but will always lead to deviations from the geo-version of a model in a specific case. It therefore remains difficult to recommend the use of several scenarios for different pesticide use situations. Such regulatory decisions should finally be based on extensive example modelling.

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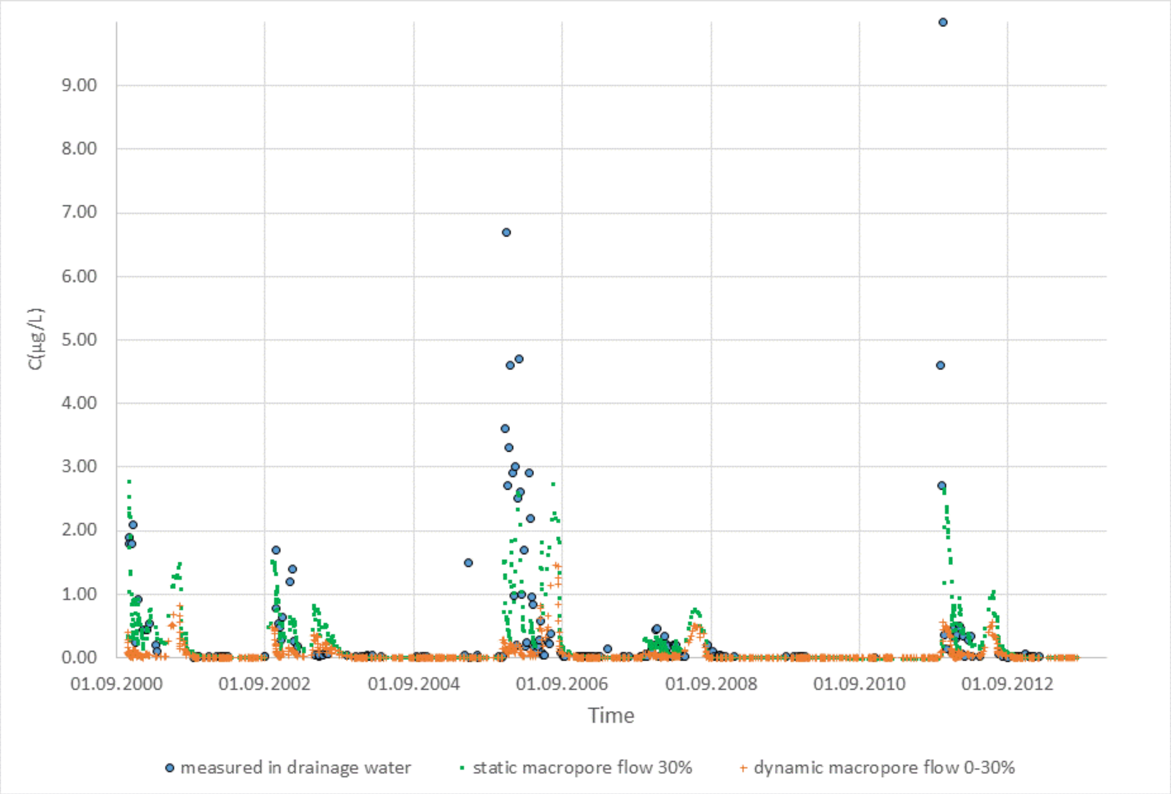
A Appendix: Additional simulations using the PLAP-dataset

Additional modelling results are provided in the following for the active substance glyphosate and its metabolite AMPA, for the active substance Fluazifop-P-butyl and its metabolites FP and TFMP as well as the active substance metribuzin and its metabolites DK and DADK by using site-specific climate and soil scenarios from the Danish PLAP monitoring system in PELMO and different modelling routines to address preferential flow as additional process for leaching. They have finally not been used to calibrate the new modelling routine for preferential flow in PELMO.

A.1 Glyphosate at Estrup

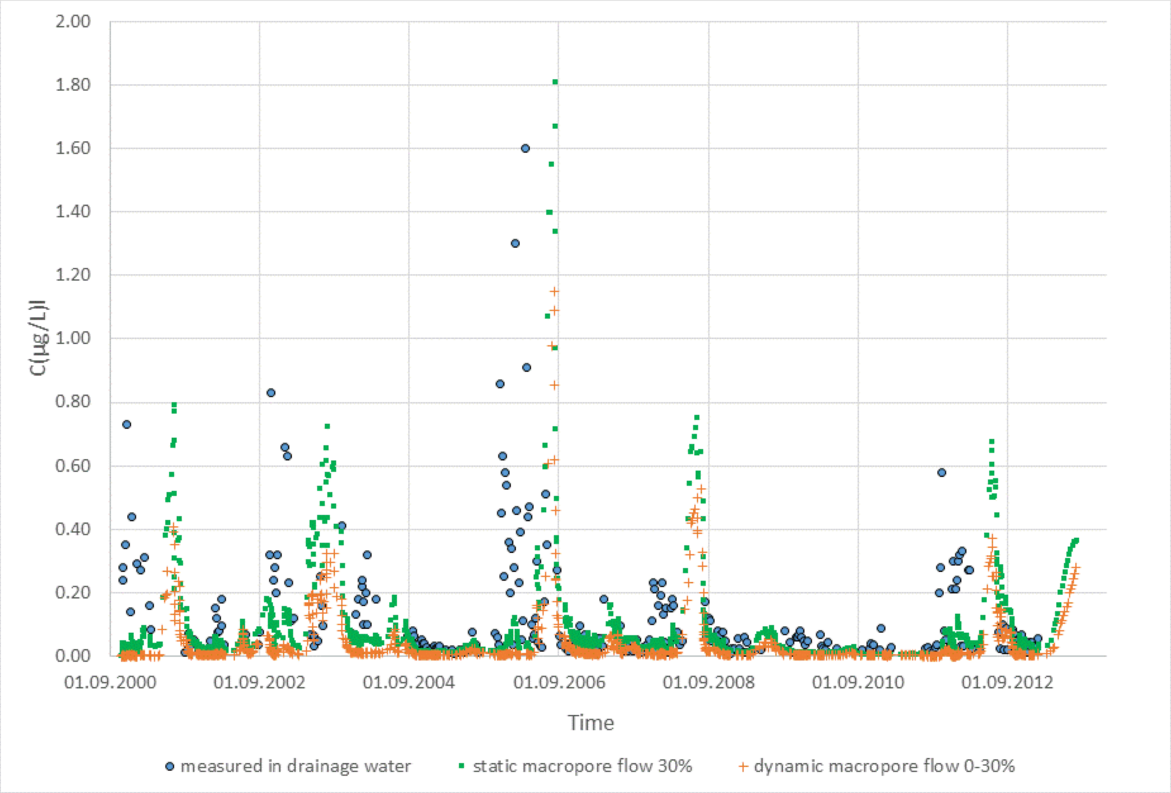
As summarised in chapter 4 glyphosate was applied six times at the PLAP site Estrup always on bare soil conditions. The nominal application rates varied between 1080 and 1440 g/ha. With the standard modelling routine in PELMO glyphosate and its metabolite AMPA are hardly transported in the soil water due to their high sorption constants. The same can be expected if preferential flow is considered as additional process. However, the PLAP dataset showed significant transport into the drainage system. In order to mimic this leaching process a special modelling routine was used which was implemented into PELMO already in 2003 (Kördel et al. 2003). In this routine the effect of dissolved organic carbon (DOC) is considered. The idea behind is that glyphosate and AMPA are bound to DOC and transported together with DOC in the soil water solution independent of their very high K_{foc} values. For the DOC content at the site Estrup 200 mg/L were set, a value which is within the expected range of DOC contents (Federer and Sticher 1994).

Figure 106: Comparison of measured and calculated glyphosate concentrations in the percolate (drainage) at 85 cm soil depth at the Danish PLAP site Estrup



Source: own illustration, Fraunhofer IME.

Figure 107: Comparison of measured and calculated AMPA concentrations in the percolate (drainage) at 85 cm soil depth at the Danish PLAP site Estrup



Source: own illustration, Fraunhofer IME.

Four different simulations were performed. First of all, the standard PELMO simulation (chromatographic flow only) and the simulation with an increased dispersion length were both not able to reproduce any measured concentrations in the percolate and they were therefore not presented. The results for two variations considering the dynamic macropore flow module are presented in Figure 106 compared to measured results. The third variation based on macropore flow of 30 % showed a similar shape as measured concentrations in the experiment (blue squares). At the beginning of the simulation period, the maximum measured concentrations were overestimated and at the end underestimated. A similar performance was achieved when using the new dynamic preferential flow module (0-30 %) in PELMO where the fraction of substances routed through macropores depend on actual soil moisture conditions of the past week. During most of the simulation period the height of measured concentrations was simulated well, but the peaks were underestimated.

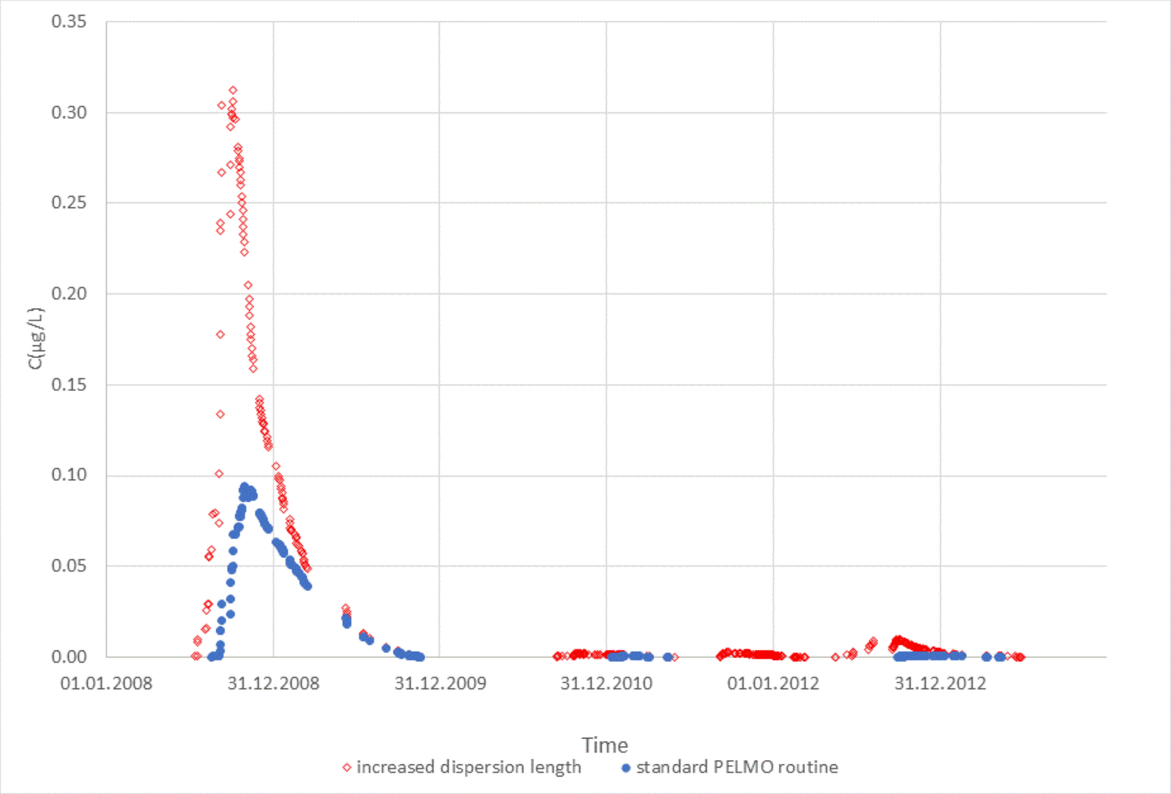
The respective results for the metabolite AMPA are presented in Figure 107. The results for the standard PELMO simulation (chromatographic flow only) and the simulation with an increased dispersion length are not presented since no substance in the percolate was simulated. The simulations using the two different variations of the macropore flow module in PELMO (static and dynamic macropore flow) both simulated concentrations in a comparable range compared to the experimental data. However, the timings of the peak concentrations were often not met because in the PELMO simulation the maximum concentrations were simulated some weeks later. According to the input data, AMPA needs a few weeks to be formed from glyphosate. Therefore, the fast formation of the metabolite AMPA at the site Estrup is difficult to reproduce with the model and it is not surprising that the model finally calculates maximum concentrations at a later stage. However, the simulated concentrations with both macropore flow variations are still in a comparable range compared to the measured field data.

A.2 Fluazifop-P-butyl at Silstrup

According to the classification scheme for macropore flow, the soil profile at the PLAP site Silstrup belongs to the same class as the Estrup soil profile (class 3: high macropore flow, soils with > 30 % clay). Therefore, as an initial step the same setting for the quantity of macropore flow was considered for the site Silstrup as for Estrup.

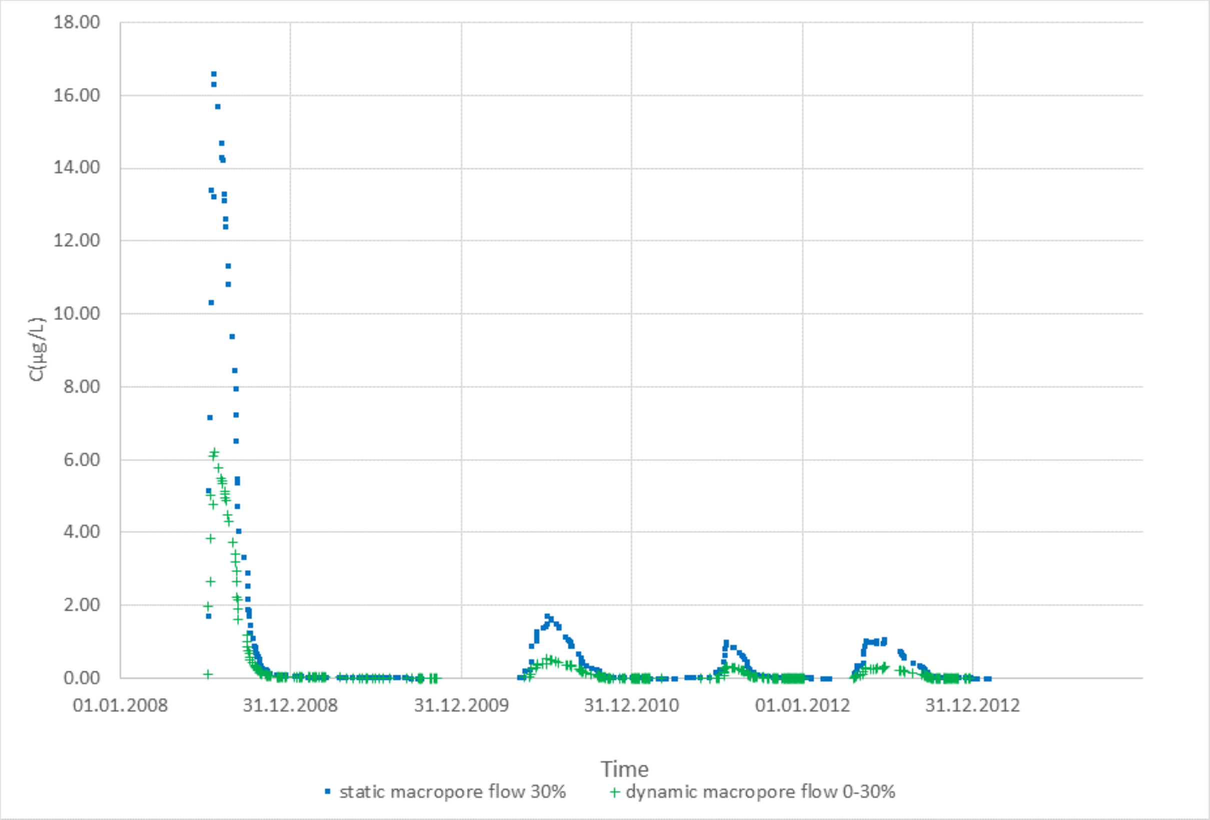
As summarised in chapter 4 fluazifop-P-butyl was applied four times at the PLAP site Silstrup to sugar beet and grass between 2008 and 2012. The nominal application rates varied between 188 and 375 g/ha. The recommended crop interception was 20 % and 90 % for the application in sugar beet and grass, respectively. In order to realistically simulate the fate of the compound the pesticide was applied to the canopy and wash-off was considered in the PELMO simulations. In contrast to the active substances glyphosate and azoxystrobin at Estrup, the parent compound fluazifop-P-butyl and the first metabolite were never observed in the drainage system. Consequently, the effect of dissolved organic carbon (DOC) as additional transport process was not considered. The fate of fluazifop-P-butyl and the two metabolites FP and TFMP were simulated. Again, four different PELMO variations were performed. Finally, the active substance fluazifop-P-butyl was not simulated in any of the model variations. That is in line with the observations at the site Silstrup.

Figure 108: Comparison of calculated concentrations of metabolite FP in the percolate (drainage) at 100 cm soil depth at the Danish PLAP site Silstrup with the standard PELMO routine and an increased dispersion length



Source: own illustration, Fraunhofer IME.

Figure 109: **Comparison of calculated concentrations of the metabolite FP in the percolate (drainage) at 100 cm soil depth at the Danish PLAP site Silstrup with two variations of the macropore flow module in PELMO**



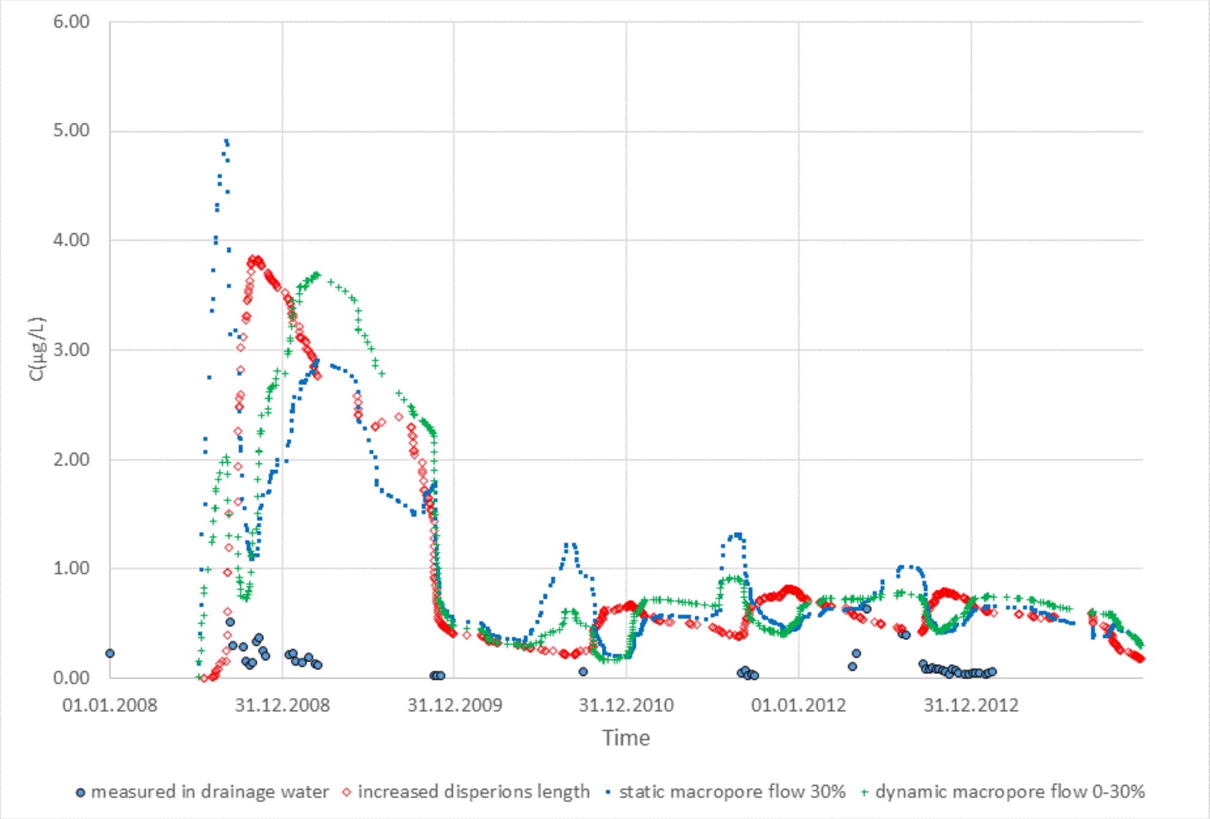
Source: own illustration, Fraunhofer IME.

The metabolite FP was not detected during the experiment, but FP was simulated in all PELMO variations (standard simulation considering chromatographic flow and various variations considering preferential flow in addition). The results for two model variations with standard PELMO simulation and an increased dispersion length are presented in Figure 108, and concentrations up to 0.08 µg/L and 0.3 µg/L were simulated after the first application in 2008. Significant higher concentrations up to 0.6 µg/L and 14 µg/L were simulated for the static and dynamic macropore flow variation, respectively (see Figure 109). The main reason for this outcome is the low organic carbon content of the Silstrup soil profile (< 0.3 % below 30 cm). That can be considered as realistic worst-case situation with regard to leaching conditions even when only chromatographic flow conditions are assumed by modelling. Nevertheless, in the experiment no FP was measured in the drainage. A reasonable explanation could be that various worst-case assumptions are taken in the model simulation (*e.g.*, the extreme short half-life of 0.3 days for fluazifop-P-butyl which leads to fast metabolite formation).

The respective results for the second metabolite TFMP are presented in Figure 110. All PELMO simulations led to similar concentrations in the percolate at 100 cm soil depth: Maximum concentrations of about 4 µg/L were simulated in 2008 after the application in sugar beet. For the rest of the simulation period (application to grass) concentrations were about 0.5 µg/L due to the lower application rate and the high crop interception of 90%. However, none of the PELMO variations could mimic what was measured in the drainage under field conditions: maximum concentrations of TFMP were only about 0.5 µg/L in 2008 and 2012. During the rest of the monitoring period concentrations were below the trigger value of 0.1 µg/L. It is most reasonable that this is a consequence of the bad performance of the simulation of its precursor metabolite FP (concentrations between 4 µg/L and 20 µg/L dependent on the PELMO variation but below detection limit during the monitoring).

Overall, it can be concluded that based on the very low organic carbon content in the Silstrup soil profile together with standard parameter setting for the substance and application properties PELMO is able to sufficiently predict conservative leaching concentrations based on the standard chromatographic flow modules in PELMO. Under these conditions the different preferential flow modules in PELMO only lead to slightly higher leaching concentrations (see Figure 110). Therefore, no additional simulations were performed with a reduced macropore flow fraction like for axzoxystrobin at the site Estrup.

Figure 110: Comparison of calculated concentrations of the metabolite TFMP in the percolate (drainage) at 100 cm soil depth at the Danish PLAP site Silstrup with two variations of the macropore flow module in PELMO



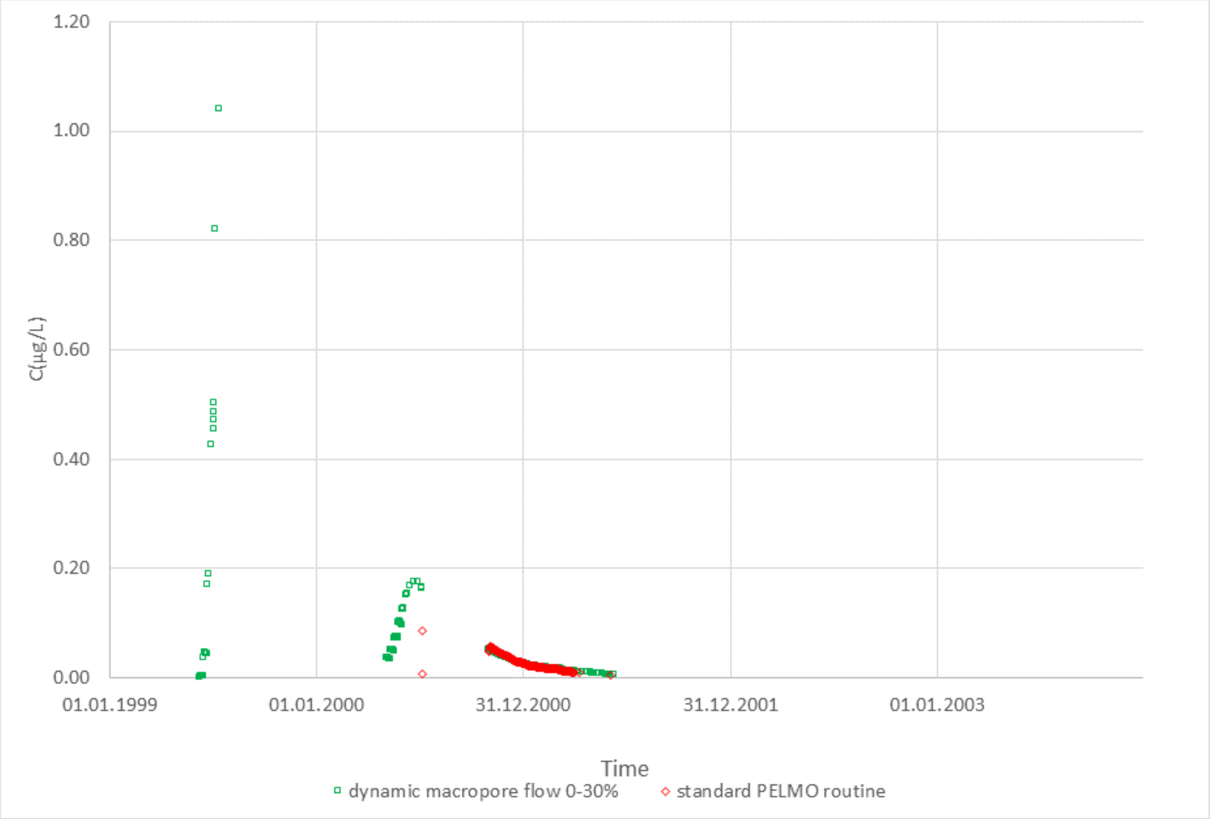
Source: own illustration, Fraunhofer IME.

A.3 Metribuzin at Tylstrup

As summarised in chapter 4 metribuzin was applied 2 times at the Danish PLAP site Tylstrup to potatoes in 2009 (140 g/ha and 105 g/ha). Crop interception was not considered (applications at BBCH 0). The fate and exposure of the active substance metribuzin and its four metabolites U1, DK, DA and DADK were simulated. Because the soil profile at Tylstrup is very sandy, it is unlikely that leaching through macropores play an important role. Nevertheless, the macropore flow module was still used in the simulation but the fraction of water routed through the macropore domain was set to a minimum value of 0.05 (5 %). In addition, also a standard PELMO simulation was performed considering only chromatographic flow. The effect of dissolved organic carbon (DOC) as additional transport process was not considered for the PELMO simulations because the five compounds are not characterised by strong sorption.

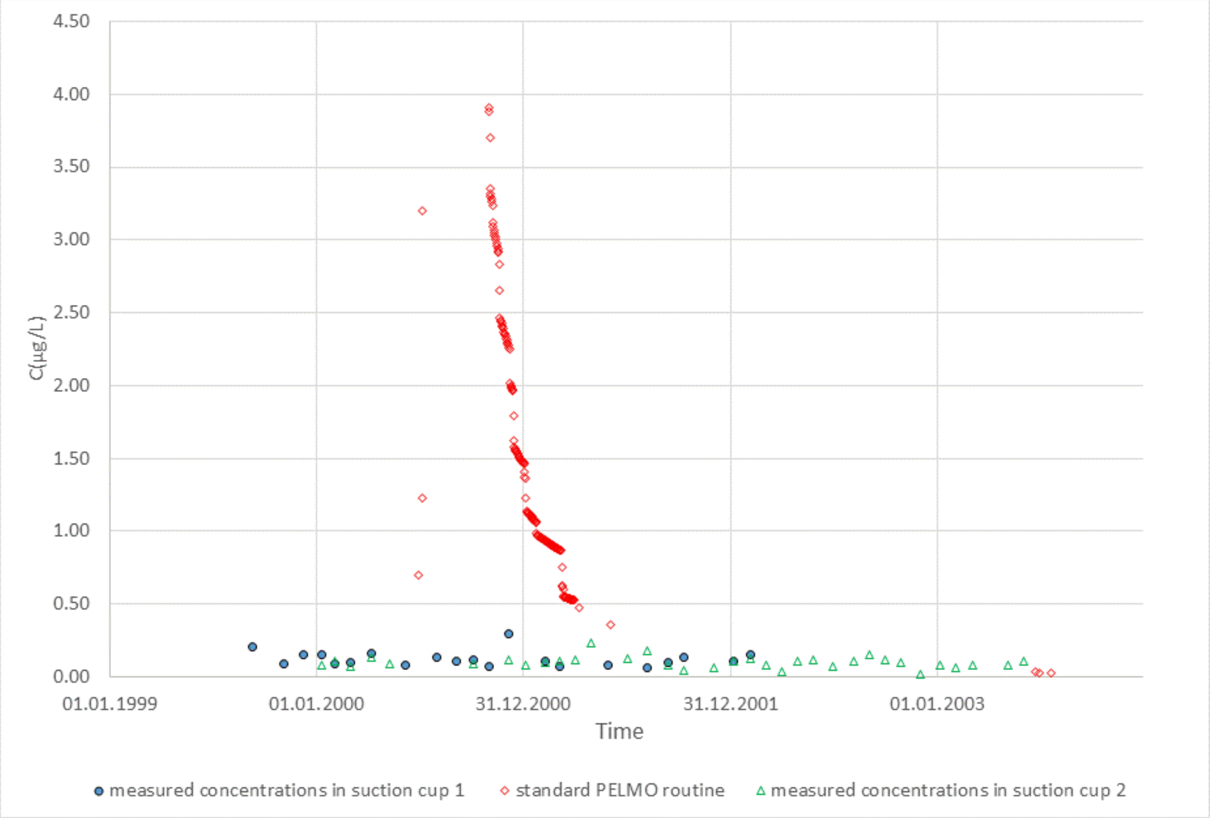
Metribuzin was observed in only three soil water samples in the range of 0.01 µg/L to 0.02 µg/L, but the active substance was simulated in both PELMO simulations with and without macropore flow as shown in Figure 111. In the standard PELMO simulation (only chromatographic flow) maximum concentrations of about 0.09 µg/L were simulated one year after application. The simulation considering macropore flow resulted in concentrations of 1.6 µg/L directly after application and 0.2 µg/L in the second year. Obviously, the standard PELMO simulation resulted in slightly more conservative results than observed in the field. However, the trigger value of 0.1 µg/L was not reached in the simulation. The soil profile at site Tylstrup is characterised by a very low organic carbon content below 60 cm soil depth. The deviations between the monitoring and PELMO calculation might be explained by the sensitivity of this parameter for the estimation of percolate concentrations in deeper soil layers. In contrast, the simulation considering dynamic macropore flow significantly overestimated the leaching of metribuzin. However, a site with a sandy soil like Tylstrup would finally be classified as 'no macropore flow' in GeoPELMO DE.

Figure 111: Comparison of calculated metribuzin concentrations in the soil at 100 cm soil depth at the Danish PLAP site Tylstrup (standard PELMO simulation and simulation with dynamic macro pores, metribuzin not detected in the experiment)



Source: own illustration, Fraunhofer IME.

Figure 112: **Comparison of measured and calculated DK concentrations in the soil at 100 cm soil depth at the Danish PLAP site Tylstrup**

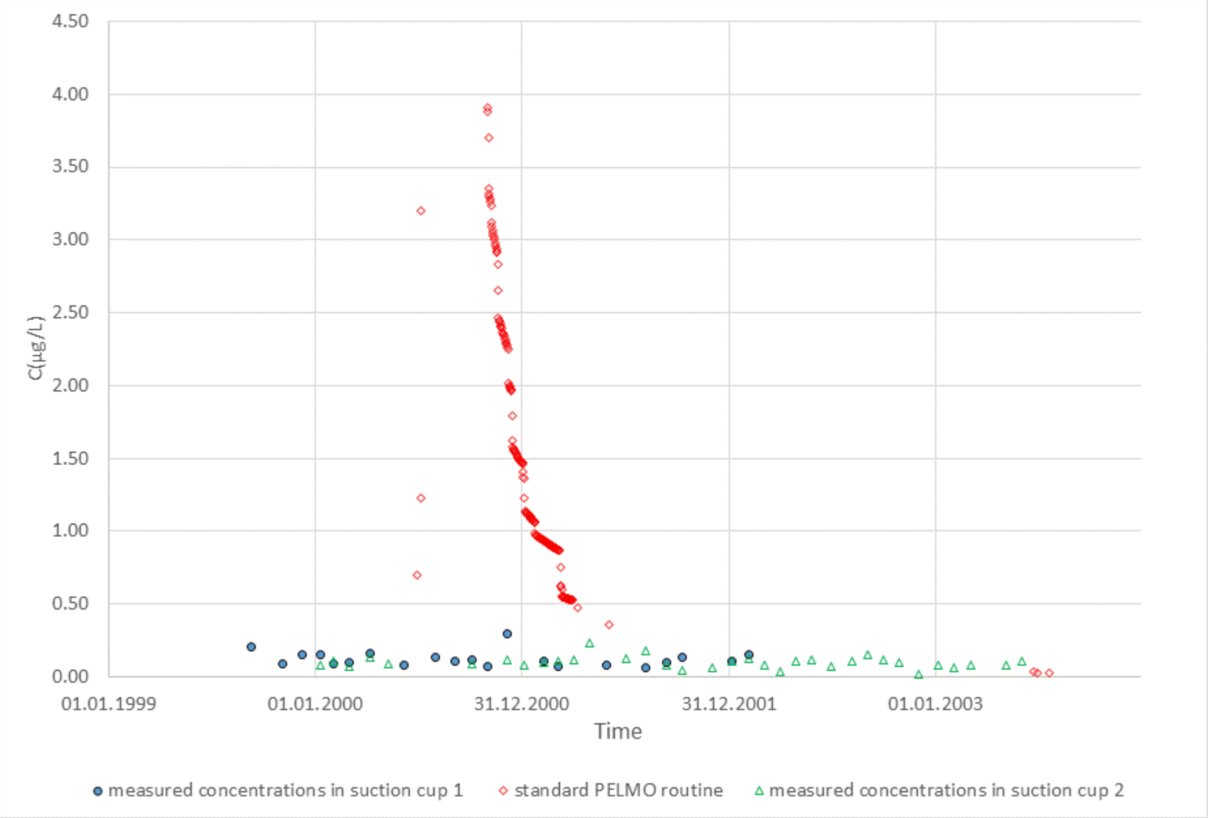


Source: own illustration, Fraunhofer IME.

The concentrations of metabolite DK at 1 m soil depth were overestimated by PELMO as shown in Figure 112 independent of the consideration of macropore flow. Whereas at both sampling points (S1 and S2) maximum concentrations of 0.5 µg/L were detected, the standard PELMO simulation (chromatographic flow only) predicted a higher steep peak of 4 µg/L about 1 year after application. Obviously, the model was neither able to estimate the maximum nor the average concentrations: the maximum concentrations (peak) were underestimated whereas the average concentrations (time before and after the peak) were underestimated. Looking at the other PELMO simulation using macropore flow in addition, at least the shape of the concentration curve was slightly better since concentrations above 0.1 µg/L were simulated not only for a short peak but for a longer time. However, the level of these concentrations was overestimated. Nevertheless, the shape of the measured results over time indicates that some macropore flow was occurring at Tylstrup although the simulation could not completely reproduce the detections based on the simple preferential flow module in PELMO.

The results for the second metabolite DADK are presented in Figure 113. Maximum concentrations of 2 µg/L were detected in the monitoring about one year after the applications. During most of the experimental period concentrations in the range of 0.1 µg/L to 0.5 µg/L were measured. The standard PELMO model (chromatographic flow) overestimated the maximum concentration (7.5 µg/L) and calculated a breakthrough few months later. Apart from the peak in winter 2000/2001 the concentration in 100 cm soil depth were near zero. The PELMO variation considering dynamic macropore flow estimated a slightly earlier breakthrough and low DADK concentrations also before and after the maximum concentration of 6 µg/L in winter 2000/2001. Hence, this simulation represents better the experimental conditions at Tylstrup. However, deviations between measured and simulated detections remain significant. To reduce those deviations, further calibrations of soil hydrologic parameters or site-specific fate parameters (*e.g.,* degradation rates, formation fractions, sorption constants) would be needed.

Figure 113: Comparison of measured and calculated DADK concentrations in the soil at 100 cm soil depth at the Danish PLAP site Tylstrup



Source: own illustration, Fraunhofer IME.

A.4 Comparison of long-term simulations (80th percentiles) using the PLAP site scenarios with results from the FOCUS scenario Hamburg

The intention of this comparison is to analyse whether the PELMO modules which simulate preferential flow predict leaching in an acceptable range when comparing the 80th temporal percentile of annual percolate concentrations at 1 m soil depth considering simulation periods over 26 years. Measured and modelled results for different PLAP sites (Estrup, Silstrup and Tylstrup) are compared with each other and with results for the FOCUS Hamburg scenario. Estrup and Silstrup represent sites with silt and clay soils which are characterised by preferential flow pattern. Tylstrup represents a site with typical leaching under sandy soils. This analysis shall also indicate if modelling results from the FOCUS Hamburg scenario are able to cover typical sites with preferential flow pattern.

In Table 101 results from standard PELMO simulations for the FOCUS Hamburg scenario are presented together with results from four different PELMO variations for different PLAP locations:

- standard FOCUS routines (chromatographic flow)
- increased dispersion length (chromatographic flow)

- static macropore flow (chromatographic + preferential flow)
- dynamic macropore flow (chromatographic + preferential flow)

In addition, Table 101 presents the measured concentrations (in groundwater and in drainage water at 1 m soil depth). For a better comparison, the measured concentrations in drainage are provided as 80th temporal percentiles of all measured concentrations for one compound at one site.

For these long-term simulations weather data from the MARS-climate database was considered for the PLAP sites in Denmark. Rainfall data was scaled.

Azoxystrobin was detected in drainage only below the trigger of 0.1 µg/L but PELMO calculated similar results in three of the four model variations. Even the simulation run based on FOCUS chromatographic flow was in line with the monitoring results. Obviously, the high amount of annual precipitation together with low amounts of organic carbon in soil could already explain the azoxystrobin leaching at Estrup and at Silstrup. Only the model variation with static macropore flow slightly overestimated the azoxystrobin transport in soil at both locations.

The PELMO results for the metabolite CyPM at Silstrup were also in line with the observations in the drainage water. However, at the site Estrup the measured 80th percentile concentration of 0.156 µg/L was not met by any of the PELMO model variations. The estimated 80th percentile concentration were always below 0.1 µg/L.

For glyphosate and AMPA at Estrup two PELMO simulations (static and dynamic macropore flow) correctly simulated concentrations above the trigger value of 0.1 µg/L. The other two model variations considering the standard FOCUS routines and an increased dispersion length as well as the results for the FOCUS Hamburg scenario did not cover the real transport of glyphosate and AMPA in the soil down to 1 m depth.

The metabolite FP of fluazifop P-butyl, which was not detected in the drainage water, was correctly simulated by all PELMO model variations and in the FOCUS Hamburg scenario. Beside the leaching of the metabolite TFMP (80th percentile if measured concentrations in drainage water: 0.136 µg/L) was correctly simulated by most of the PELMO model variations and the FOCUS Hamburg scenario. Only in the PELMO simulation based on FOCUS standard with chromatographic flow predicted a lower concentration which remained slightly below 0.1 µg/L (0.092 µg/L).

Metribuzin was observed at Tylstrup in only three soil water samples in the range of 0.01 µg/L to 0.02 µg/L. Two PELMO model variations (FOCUS standard, increased dispersion) and results for the FOCUS Hamburg scenario are in line with the measured results. Those results are reliable since the PLAP site Tylstrup represents a very sandy soil. The two remaining model variations with static and dynamic macropore flow significantly overestimated the 80th percentile measured metribuzin concentrations (static macropore flow: with two orders of magnitude, dynamic macropore flow: with one order of magnitude). It must be considered that a site like Tylstrup will not be parametrised with macropore flow in GeoPELMO DE.

The metabolites DK and DADK of metribuzin were both detected in the soil water above 0.1 µg/L. Comparable concentrations were also predicted with the FOCUS Hamburg scenario: 0.156 µg/L and 0.434 µg/L. This result is acceptable since the site Tylstrup and the FOCUS

Hamburg scenario both represent sandy soil profiles and the influence of macropore flow should be low or negligible. However, similar results were still simulated with the PELMO model variations considering macropore flow. This seems still acceptable, because only a very small fraction of macropore flow in the soil core was considered.

Conclusions of the comparison

When looking at daily concentrations none of the three macropore flow modules in PELMO could exactly reproduce the transport through preferential flow in the PLAP fields Estrup and Silstrup. Primarily, the model version with an increased dispersion length did not predict any early breakthrough like it measured. The breakthrough times were achieved much better by the static or dynamic macropore flow modules in PELMO, although the peak values were often not met. Especially, the static model variation with constant fractions of macropore flow was highly overestimating the leaching. In comparison, the dynamic model variation with macropore flow fractions in soil dependent on the soil moisture content showed the best performance when focusing on daily concentrations in drainage.

When considering aggregated concentrations (80th temporal percentiles of annual concentrations over a longer time) the differences between the results from the tested model variations became less significant. Especially, the results of the model variation with an increased dispersion length were rather similar as simulations with the two model versions with macropore flow. But due to the low organic carbon contents in the PLAP soil profiles, even simulations with the FOCUS standard routine in PELMO lead to comparable results like to the other model variations. Obviously, the aggregation of the leaching behaviour over longer time periods proofs that the total amount of compounds transported through the PLAP soils where quite similar, even when the dynamics of leaching was not exactly covered.

The leaching behaviour of glyphosate and AMPA at Estrup were exceptions in the modelling analysis. Both compounds could only be simulated well when the dynamic macropore flow module combined with transport of the compounds via DOC in soil was considered. All other model variations either overestimated the transport (static macropore flow module) or did not simulate any transport through the soil at all (FOCUS Hamburg scenario, site-specific FOCUS standard simulation, site specific calculation with an increased dispersion length). The reason is very high K_{foc} values of the active substance glyphosate and its metabolite AMPA (15388 L/kg and 9749 L/kg). Even both macropore flow modules could not simulate the transport of both compounds in the soil water, when the inclusion of the DOC-phase in the modelling was not considered.

For the selection of the macropore flow model variation, it is recommended to use the dynamic version as this variation achieved the best results when comparing with daily and aggregated concentrations.

Table 101: Comparison of annual 80th percentile concentrations in the percolate at 1 m soil depth simulated with PELMO for the PLAP sites Estrup, Silstrup and Tylstrup and the FOCUS Hamburg scenario

Active substance (as)/ metabolite (m)	PLAP site	Crop	C(µg/L) measured results PLAP		C (µg/L) FOCUS Hamburg	C (µg/L) calculated for PLAP site (annual concentration)			
			80th percentile in drainage	Groundwater*		Standard	Increased dispersion length	Static macro pore flow	Dynamic macro pore flow
Azoxystrobin (as)	Estrup	Spring cereals	0.004	(244,0,0)	0.000	0.003	0.026	0.068	0.032
CyPM (m)			0.156	(329,27,0)	0.000	0.019	0.078	0.059	0.042
Azoxystrobin (as)	Silstrup	Spring cereals	0.000	(563,2,0)	0.000	0.003	0.013	0.126	0.082
CyPM (m)			0.060	(547,17,1)	0.000	0.021	0.060	0.089	0.088
Glyphosate (as)	Estrup	Grass	0.180	(817,42,5)	0.000	0.000	0.000	0.539	0.147
AMPA (m)			0.160	(858,8,0)	0.000	0.000	0.000	0.1736	0.053
Fluazifop-P-butyl (as)	Silstrup	sugarbeet/	<LOD	-	0.000/0.000°	0.000	0.000	0.000	0.000
Fluazifop P (m)		grass	<LOD	(169,0,0)	0.002/0.000°	0.000	0.000	0.000	0.000
TFMP (m)			0.136	(225,71,16)	4.227/0.104°	0.092	0.294	1.386	0.698
Metribuzin (as)	Tylstrup	Potatoes	<LOD	(336,1,0)	0.000	0.001	0.012	1.617	0.14
DK (m)			0.150	(73,141,315)	0.156	0.184	0.453	1.079	0.211
DADK (m)			0.688	(289,234,5)	0.434	0.437	0.819	0.705	0.343

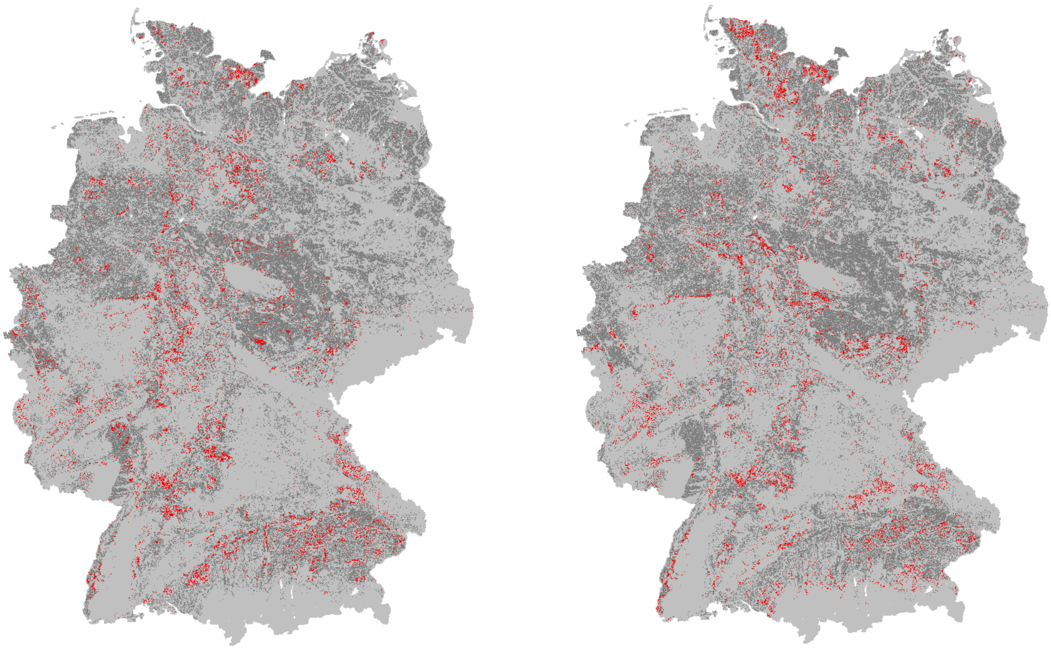
* The number of exceedances given in the brackets, for example (800, 200, 20), are the number of analyses not detected (800), the number of analyses > LOD and ≤ 0.1 µg/L (200) and the number of analyses > 0.1ug/L (20).

° sugar beet and grass application

B Appendix: Distribution of the 80 ± 5th spatial percentiles of the annual percolate concentrations from three dummy active substances and two metabolites to prepare national scenario selection

Figure 114: Distribution of the 80 ± 5th spatial percentiles of annual percolate concentrations for dummy active substance P1 in maize (left) and winter cereals (right)

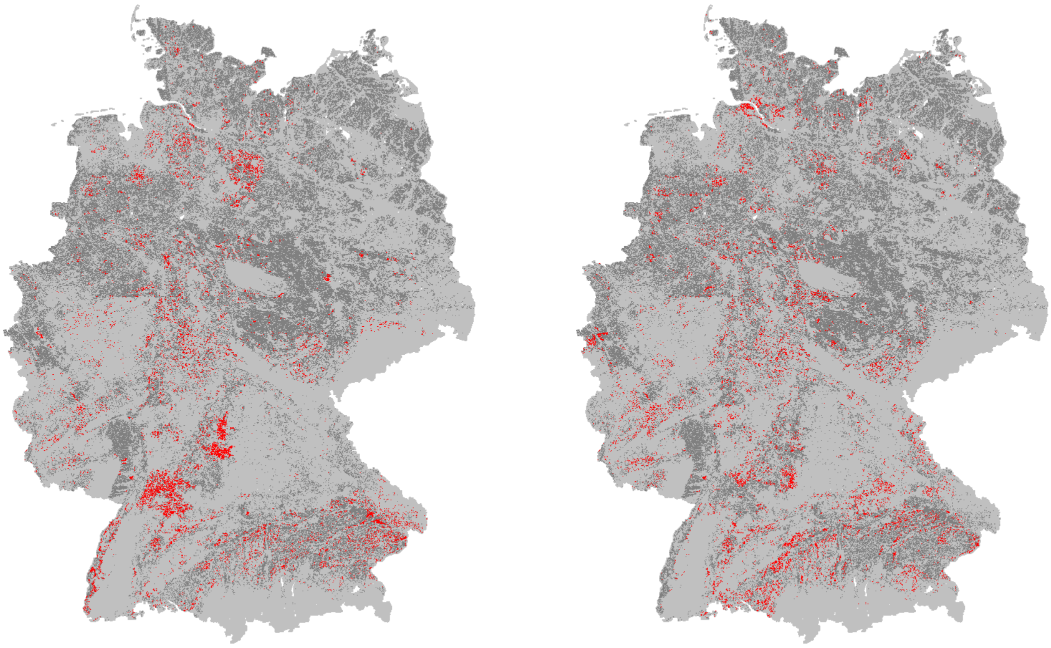
Model simulations are conducted with the GeoPELMO DE (FOCUS L+R+M+D) including runoff, macropore flow and drainage. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

Figure 115: Distribution of the 80 ± 5th spatial percentiles of annual percolate concentrations for dummy active substance P3 in maize (left) and winter cereals (right)

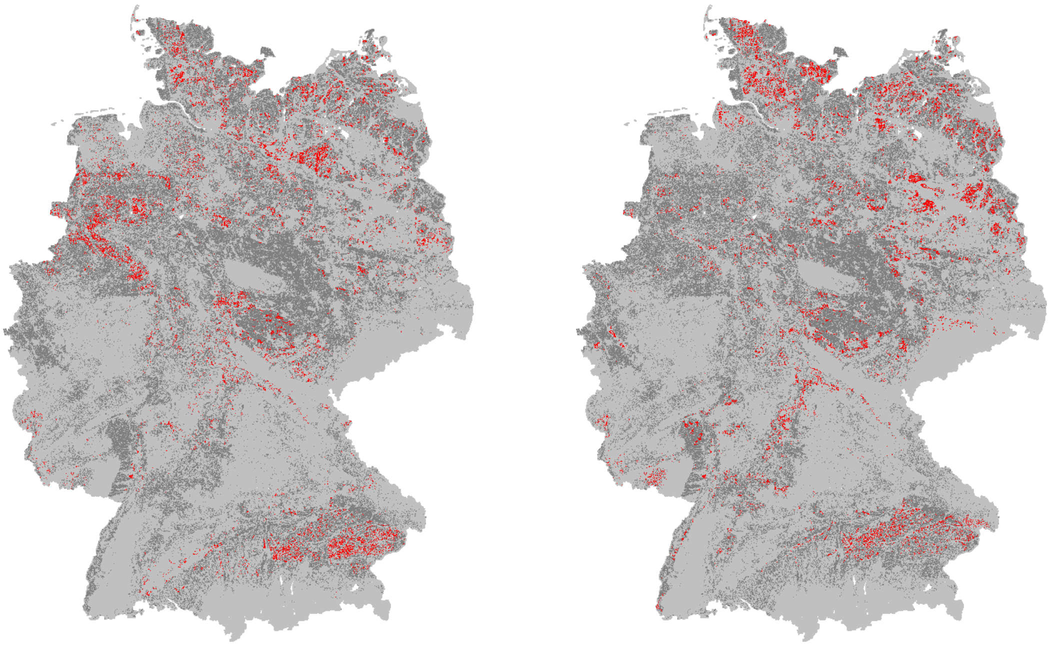
Model simulations are conducted with the GeoPELMO DE (FOCUS L+R+M+D) including runoff, macropore flow and drainage. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

Figure 116: Distribution of the 80 ± 5th spatial percentiles of annual percolate concentrations for dummy metabolite M2 formed from P1 in maize (left) and winter cereals (right)

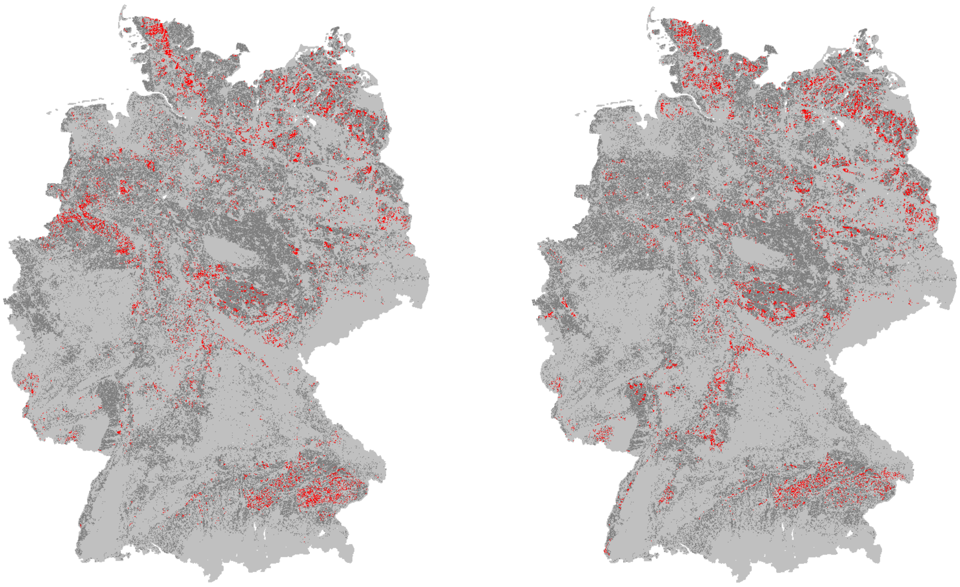
Model simulations are conducted with the GeoPELMO DE (FOCUS L+R+M+D) including runoff, macropore flow and drainage. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

Figure 117: Distribution of the 80 ± 5th spatial percentiles of annual percolate concentrations for dummy metabolite M2 formed from P2 in maize (left) and winter cereals (right)

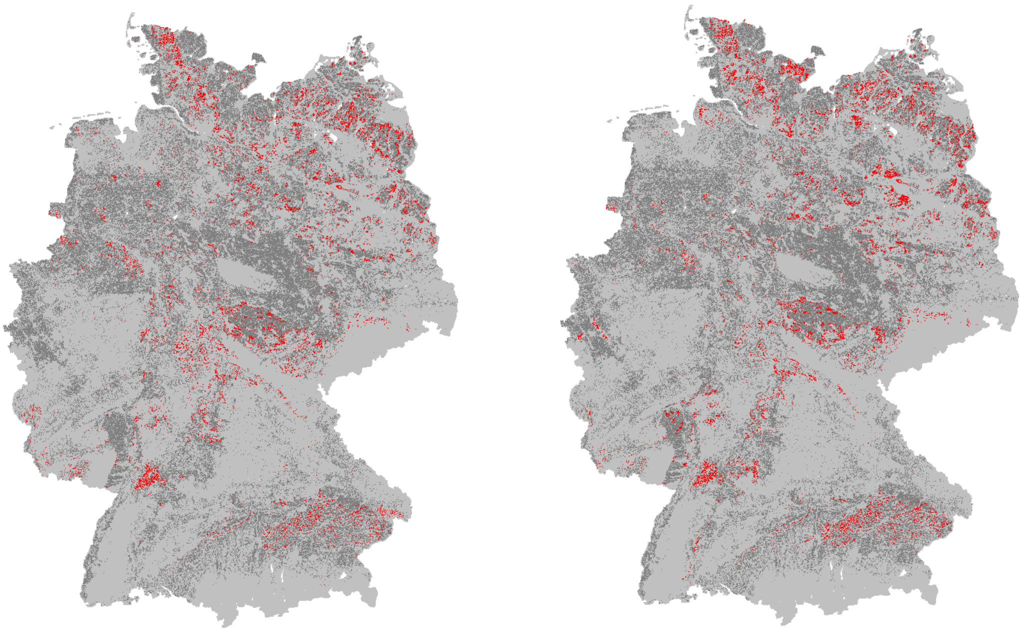
Model simulations are conducted with the GeoPELMO DE (FOCUS L+R+M+D) including runoff, macropore flow and drainage. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

Figure 118: Distribution of the 80 ± 5th spatial percentiles of annual percolate concentrations for dummy metabolite M2 formed from P3 in maize (left) and winter cereals (right)

Model simulations are conducted with the GeoPELMO DE (FOCUS L+R+M+D) including runoff, macropore flow and drainage. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010).



Source: own illustration, Fraunhofer IME.

C Appendix: Results of additional simulations with GeoPELMO DE considering further scenarios

In chapter 6, a selection and analysis of alternative scenarios derived from dummy active substance dummy metabolites was presented. Comparisons of calculated PECs from the new scenarios with the FOCUS Hamburg scenario and the 80th spatial percentiles from GeoPELMO DE were provided for real pesticide uses. In this appendix further 14 scenarios are presented based on selected climate-soil-combinations from GeoPELMO DE (version FOCUS L+R+M+D) suggested from simulation runs with real active substances and metabolites from real pesticide uses. These scenarios may also represent an approximation on the 80th percentiles for metabolites as they were mainly selected based on the results for real transformation products.

The results presented in Table 102 and Table 103 show a relative inhomogeneous distribution of percentiles for active substances ranging from 45 % (combination 610 Schleswig) to 89 % (combination 15884 Göttingen) for the average. Results for the real transformation products are summarised in Table 104 and Table 105. The distribution of the spatial percentile was found to be in the range of 41 % (combination 15254 Lübeck) to 74 % (combination 3303 Sachsenheim) for the additionally selected scenarios.

Table 102: Comparison of spatial percentiles of annual leachate concentrations from further individual climate-soil-combinations with GeoPELMO DE for eleven active substances (part 1)

Model simulations with GeoPELMO DE (FOCUS L+R+M+D) were conducted for active substances from real pesticide uses. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010). If the PEC from the scenario was calculated to be outside the spatial percentile range of 75 % to 85 %, the percentiles were estimated with an uncertainty of ±2.5 %.

Activ substance	Number of metabolites considered	610/ 216/ Schleswig [%]	1687/ 524/ Erfde [%]	6111/ 2612/ Lübeck-Blank. [%]	6129/ 2620/ Quickborn [%]	6597/ 7853/ Parsberg [%]	9521/ 3416/ Emmendingen [%]
Azoxystrobin (a)	32.5	72.5	81.4	77.4	57.5	87.5	87.5
Bentazone (b)	57.5	75.6	72.5	79.1	80.4	97.5	75.3
Chlorothalonil (c)	42.5	76.1	72.5	67.5	62.5	92.5	81.5
Clothianidin (d)	82.5	87.5	87.5	87.5	62.5	97.5	87.5
Diflufenican (e)	32.5	75.9	78.9	72.5	67.5	82.6	83.6
Flufenacet (f)	27.5	72.5	79.6	67.5	67.5	76.9	79.8
Imazamox (g)	92.5	87.5	77.3	79.4	76.8	57.5	57.5
Isoproturon (h)	32.5	72.5	83.0	79.1	62.5	83.4	72.5
Metazachlor (i)	27.5	87.5	87.5	77.8	52.5	87.5	87.5
S-Metolachlor (j)	37.5	62.5	81.2	77.8	57.5	83.0	83.1
Terbuthylazine (k)	32.5	72.5	76.4	72.5	62.5	81.7	82.6
Minimum	**28**	**63**	**73**	**68**	**53**	**58**	**58**
Arithmetic mean	**45**	**77**	**80**	**76**	**65**	**84**	**80**
Maximum	**93**	**88**	**88**	**88**	**80**	**98**	**88**

Table 103: Comparison of spatial percentiles of annual leachate concentrations from further individual climate-soil-combinations with GeoPELMO DE for eleven active substances (part 2)

Model simulations with GeoPELMO DE (FOCUS L+R+M+D) were conducted for active substances from real pesticide uses. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010). If the PEC from the scenario was calculated to be outside the spatial percentile range of 75 % to 85 %, the percentiles were estimated with an uncertainty of ±2.5 %.

Activ substance	13698/ 5496/ Hamburg [%]	15251/ 6028/ Lübeck [%]	16386/ 6433/ Schotten [%]	1680/ 519/ Schleswig [%]	3303/ 813/ Sachsenheim [%]	2410/ 644/ Ulm [%]	15884/ 6123/ Göttingen [%]
Azoxystrobin (a)	92.5	72.5	92.5	83.0	72.5	92.5	52.5
Bentazone (b)	52.5	67.5	87.5	84.0	37.5	97.5	32.5
Chlorothalonil (c)	82.1	57.5	92.5	87.5	77.7	84.2	57.5
Clothianidin (d)	72.5	92.5	67.5	97.5	42.5	92.5	37.5
Diflufenican (e)	92.5	62.5	97.5	87.5	72.5	87.5	52.5
Flufenacet (f)	92.5	62.5	97.5	87.5	67.5	72.5	57.5
Imazamox (g)	42.5	62.5	62.5	87.5	17.5	87.5	7.5
Isoproturon (h)	97.5	84.3	87.5	92.5	62.5	87.5	52.5
Metazachlor (i)	92.5	81.1	87.5	87.5	57.5	87.5	62.5
S-Metolachlor (j)	92.5	83.6	84.7	87.5	67.5	97.5	62.5
Terbuthyl-azine (k)	92.5	77.1	92.5	77.4	67.5	97.5	57.5
Minimum	**43**	**58**	**63**	**77**	**18**	**73**	**8**
Arithmetic mean	**80**	**82**	**73**	**86**	**87**	**58**	**89**
Maximum	**98**	**93**	**98**	**98**	**78**	**98**	**63**

Table 104: Comparison of spatial percentiles of annual leachate concentrations from further individual climate-soil-combinations with GeoPELMO DE for 34 real metabolites (part 1)

Model simulations with GeoPELMO DE (FOCUS L+R+M+D) were conducted for main metabolites from real pesticide uses. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010). If the PEC from the scenario was calculated to be outside the spatial percentile range of 75 % to 85 %, the percentiles were estimated with an uncertainty of ±2.5 %.

Metabolites	610/ 216/ Schleswig [%]	1687/ 524/ Erfde [%]	6111/ 2612/ Lübeck-Blank. [%]	6129/ 2620/ Quickborn [%]	6597/ 7853/ Parsberg [%]	9521/ 3416/ Emmendingen [%]	610/ 216/ Schleswig [%]
CyPM (a)	77.9	87.5	82.9	92.5	62.5	87.5	84.5
N-methyl-bentazone (b)	32.5	62.5	67.5	87.5	62.5	97.5	87.5
R182281 (c)	47.5	87.5	77.3	87.5	52.5	92.5	87.5
R417888 (c)	27.5	17.5	42.5	32.5	32.5	47.5	52.5
R419492 (c)	27.5	12.5	42.5	32.5	27.5	42.5	47.5
MNG (d)	67.5	67.5	78.0	57.5	57.5	77.1	77.9
TZNG (d)	79.2	87.5	87.5	87.5	57.5	97.5	92.5
NTG (d)	37.5	37.5	82.5	22.5	47.5	82.5	82.5
AE 0542291 (e)	27.5	72.5	82.0	72.5	62.5	82.7	87.5
AE B107137 (e)	47.5	83.9	77.8	85.0	57.5	72.5	79.1
FOE Thiadone (f)	27.5	72.5	78.4	67.5	67.5	76.1	80.3
TFA (f)	17.5	12.5	47.5	32.5	17.5	42.5	32.5
CL 312622 (g)	92.5	92.5	77.6	92.5	62.5	72.5	72.5
CL 354825 (g)	42.5	72.5	83.6	92.5	42.5	97.5	97.5
Desmethyl-IPU (h)	42.5	81.6	77.2	79.7	62.5	87.5	80.7
Didesmethyl-IPU (h)	47.5	22.5	67.5	47.5	52.5	52.5	67.5
1-OH-IPU (h)	83.4	87.5	72.5	67.5	82.8	57.5	47.5
2-OH-IPU (h)	83.3	87.5	72.5	67.5	84.1	57.5	47.5
479M04 (i)	57.5	57.5	67.5	47.5	57.5	52.5	57.5
479M08 (i)	37.5	42.5	72.5	47.5	52.5	67.5	57.5
479M09 (i)	78.5	79.2	72.5	72.5	72.5	42.5	62.5
479M011 (i)	87.5	92.5	78.4	83.6	72.5	72.5	77.6
NOA436611 (j)	32.5	22.5	57.5	37.5	37.5	62.5	62.5
ESA (j)	22.5	12.5	52.5	32.5	32.5	52.5	57.5
CGA368208 (j)	17.5	7.5	57.5	27.5	42.5	72.5	72.5

Metabolites	**610/ 216/ Schleswig [%]**	**1687/ 524/ Erfde [%]**	**6111/ 2612/ Lübeck-Blank. [%]**	**6129/ 2620/ Quickborn [%]**	**6597/ 7853/ Parsberg [%]**	**9521/ 3416/ Emmendingen [%]**	**610/ 216/ Schleswig [%]**
OXA (j)	37.5	27.5	62.5	42.5	42.5	67.5	67.5
CGA37735 (j)	22.5	17.5	67.5	42.5	37.5	72.5	77.5
CGA40172 (j)	42.5	72.5	72.5	87.5	47.5	87.5	79.6
CGA50720 (j)	37.5	22.5	62.5	32.5	57.5	57.5	57.5
MT13 (k)	72.5	72.5	82.6	83.4	47.5	83.7	87.5
MT1 (k)	76.6	92.5	81.7	92.5	62.5	82.5	80.6
MT14 (k)	83.2	87.5	82.5	92.5	62.5	82.5	82.5
LM5 (k)	72.5	67.5	82.5	67.5	67.5	72.5	77.5
LM6 (k)	17.5	12.5	52.5	27.5	47.5	72.5	67.5
Minimum	**8**	**43**	**23**	**18**	**43**	**33**	**18**
Arithmetic mean	**57**	**71**	**62**	**54**	**71**	**71**	**50**
Maximum	**93**	**88**	**93**	**84**	**98**	**98**	**93**

Table 105: **Comparison of spatial percentiles of annual leachate concentrations from further individual climate-soil-combinations with GeoPELMO DE for 34 real metabolites (part 2)**

Model simulations with GeoPELMO DE (FOCUS L+R+M+D) were conducted for main metabolites from real pesticide uses. Results are based on the 80th temporal percentiles from 20 weather years (1991-2010). If the PEC from the scenario was calculated to be outside the spatial percentile range of 75 % to 85 %, the percentiles were estimated with an uncertainty of ±2.5 %.

Metabolites	**13698/ 5496/ Hamburg [%]**	**15251/ 6028/ Lübeck [%]**	**16386/ 6433/ Schotten [%]**	**1680/ 519/ Schleswig [%]**	**3303/ 813/ Sachsenheim [%]**	**2410/ 644/ Ulm [%]**	**15884/ 6123/ Göttingen [%]**
CyPM (a)	87.5	79.4	97.5	52.5	87.5	62.5	80.2
N-methyl-bentazone (b)	67.5	87.5	87.5	67.5	92.5	52.5	82.0
R182281 (c)	80.2	79.9	97.5	67.5	87.5	57.5	87.5
R417888 (c)	57.5	2.5	22.5	52.5	52.5	80.0	37.5
R419492 (c)	47.5	2.5	17.5	52.5	52.5	82.2	32.5
MNG (d)	78.5	17.5	62.5	27.5	81.2	62.5	52.5
TZNG (d)	92.5	67.5	97.5	47.5	92.5	37.5	75.2
NTG (d)	82.5	7.5	32.5	37.5	87.5	87.5	42.5

Metabolites	**13698/ 5496/ Hamburg [%]**	**15251/ 6028/ Lübeck [%]**	**16386/ 6433/ Schotten [%]**	**1680/ 519/ Schleswig [%]**	**3303/ 813/ Sachsenheim [%]**	**2410/ 644/ Ulm [%]**	**15884/ 6123/ Göttingen [%]**
AE 0542291 (e)	72.5	92.5	84.0	67.5	92.5	57.5	97.5
AE B107137 (e)	80.8	83.4	97.5	47.5	84.5	47.5	87.5
FOE Thiadone (f)	67.5	97.5	83.2	72.5	72.5	57.5	92.5
TFA (f)	52.5	7.5	12.5	57.5	52.5	87.5	42.5
CL 312622 (g)	79.4	62.5	92.5	17.5	79.8	12.5	52.5
CL 354825 (g)	84.4	78.5	87.5	67.5	81.4	17.5	84.5
Desmethyl-IPU (h)	79.6	87.5	97.5	52.5	72.5	47.5	87.5
Didesmethyl-IPU (h)	72.5	2.5	17.5	22.5	78.6	72.5	17.5
1-OH-IPU (h)	57.5	62.5	87.5	27.5	72.5	12.5	47.5
2-OH-IPU (h)	62.5	67.5	87.5	27.5	77.0	12.5	52.5
479M04 (i)	72.5	7.5	52.5	22.5	72.5	47.5	22.5
479M08 (i)	82.5	7.5	37.5	42.5	79.7	82.5	27.5
479M09 (i)	67.5	37.5	78.6	12.5	80.1	12.5	32.5
479M011 (i)	78.4	62.5	92.5	22.5	82.9	22.5	57.5
NOA436611 (j)	62.5	2.5	27.5	52.5	52.5	80.0	27.5
ESA (j)	57.5	7.5	17.5	57.5	47.5	82.6	22.5
CGA368208 (j)	67.5	12.5	7.5	80.0	52.5	92.5	37.5
OXA (j)	72.5	7.5	32.5	47.5	57.5	78.3	27.5
CGA37735 (j)	72.5	7.5	27.5	78.2	62.5	92.5	32.5
CGA40172 (j)	79.1	87.5	97.5	72.5	87.5	57.5	92.5
CGA50720 (j)	62.5	2.5	17.5	37.5	52.5	77.5	17.5
MT13 (k)	87.5	22.5	72.5	42.5	87.5	67.5	67.5
MT1 (k)	85.0	72.5	97.5	47.5	92.5	52.5	87.5
MT14 (k)	92.5	57.5	97.5	17.5	92.5	17.5	72.5
LM5 (k)	82.5	7.5	57.5	7.5	87.5	17.5	32.5
LM6 (k)	67.5	12.5	12.5	82.1	42.5	92.5	42.5
Minimum	**48**	**3**	**8**	**8**	**43**	**13**	**18**
Arithmetic mean	**73**	**41**	**61**	**47**	**74**	**56**	**54**
Maximum	**93**	**98**	**98**	**82**	**93**	**93**	**98**

D Appendix D: Properties of active substances and metabolites used to analyse regulatory consequences of the new groundwater risk assessment approach

In chapter 6 possible consequences of the proposed alternative scenarios and modelling approaches for the lower tier national groundwater risk assessment were discussed. Eleven active substances and 34 metabolites from real pesticide uses were used to analyse the level of protection from the current FOCUS Hamburg scenario and new national climate-soil-combinations in relation to nationwide concentrations from GeoPELMO DE. In this appendix, relevant properties of the simulated compounds (active substances and their main metabolites, status quo from 2020) are summarised in Table 106. The metabolism schemes are presented below in Figures.

Table 106: Properties of the active substances and metabolites considered in the analysis

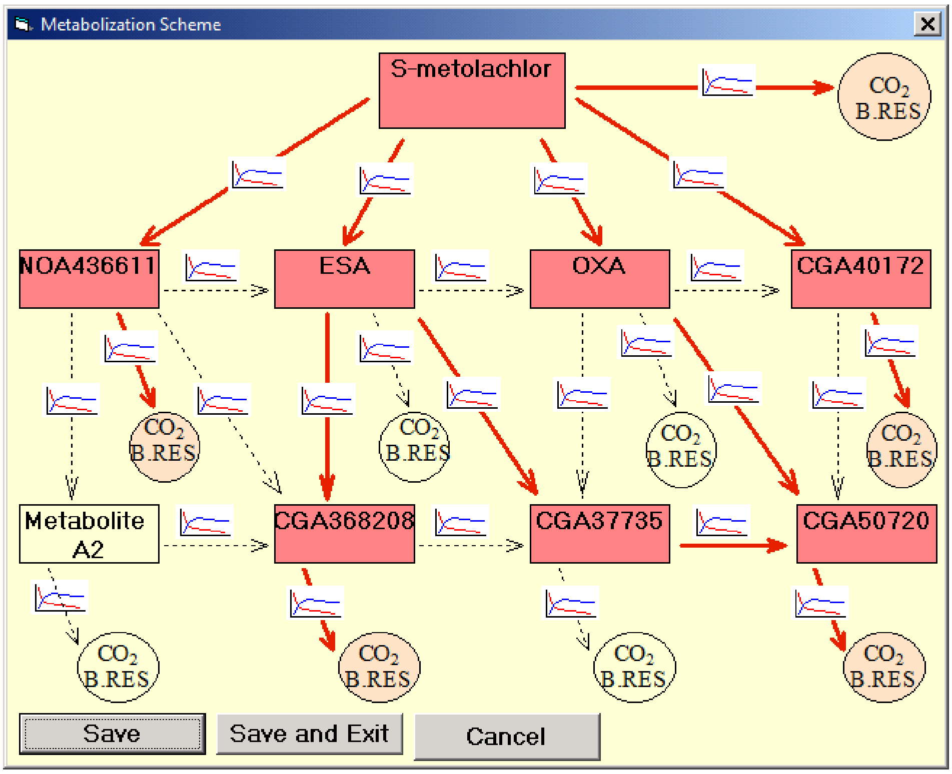
Compound	Active substance/ Metabolite	Molar mass [g/mol]	Formation Fraction [-]	DegT$_{50}$ [d]	K$_{foc}$ [L/kg]	Freundlich 1/n [-]
S-metolachlor	active substance	283.8	-	21.7	200.24	0.93
NOA436611	metabolite	355.45	0.07 (from as)	164.9	8.43	0.82
ESA	metabolite	329.4	0.11 (from as)	235	6.74	0.9
OXA	metabolite	279.3	0.13 (from as)	152	12.34	0.84
CGA40172	metabolite	265.3	0.07 (from as)	133.3	174.45	0.76
CGA368208	metabolite	257.3	0.48 (from ESA)	36.9	1.0	1.0
CGA37735	metabolite	193.2	0.52 (from ESA)	0.8	10.35	0.96
CGA50720	metabolite	207.2	1.0 (from OXA) 1.0 (from CGA37735)	10.4	1.0	1.0
Isoproturon (IPU)	active substance	206.3	-	7.8	81	0.879
Desmethyl-IPU	metabolite	192.3	0.24 (from as)	23.1	129	0.823
1-OH-IPU	metabolite	222.29	0.22 (from as)	7.9	12	0.912
2-OH-IPU	metabolite	222.29	0.11 (from as)	6.3	12	0.912

Compound	**Active substance/ Metabolite**	**Molar mass [g/mol]**	**Formation Fraction [-]**	**DegT$_{50}$ [d]**	**K$_{foc}$ [L/kg]**	**Freund-lich 1/n [-]**
Didesmethyl-IPU	metabolite	178.24	0.28 (from desmethyl-IPU)	78.1	1.0	1.0
Diflufenican	active substance	394.3	-	143.2	3417	0.917
AE B107137	metabolite	283	0.33 (from as) 1.0 (from AE 0542291)	10.6	13	0.73
AE 0542291	metabolite	282	0.37 (from as)	26.9	132	0.82
Bentazone	active substance	240.3	-	7.5	30.2	0.97
N-methyl-bentazone	metabolite	245.3	0.057 (from as)	55.8	257.5	0.868
Terbuthylazine	active substance	229.7	-	20	151	0.93
LM5	metabolite	184	0.47 (from MT14)	47	15.3	0.86
LM6	metabolite	198	0.41 (from LM5)	241	13.3	0.91
MT13	metabolite	211.28	0.197 (from as)	453	187	0.91
MT1	metabolite	201.67	0.44 (from as)	26.8	77	0.89
MT14	metabolite	183.22	0.28 (from MT1)	107	111	0.92
Clothianidin	active substance	249.7	-	253.4	124	0.81
MNG	metabolite	118.1	0.267 (from as)	114	16.5	0.859
NTG	metabolite	104.1	1.0 (from MNG) 1.0 (from TZNG)	94.7	16	0.877
TZNG	metabolite	235.7	0.181 (from as)	116.6	266.8	0.799
Chlorothalonil	active substance	265.9	-	2.9	1403	0.87

Compound	**Active substance/ Metabolite**	**Molar mass [g/mol]**	**Formation Fraction [-]**	**DegT$_{50}$ [d]**	**K$_{foc}$ [L/kg]**	**Freund-lich 1/n [-]**
R182281	metabolite (prim)	247.5	0.186 (from as)	143.9	386	0.88
R417888	metabolite (prim)	329.5	0.108 (from as)	332	9.5	1.01
R419492	metabolite (prim + sec)	357.2	0.092 (from as) 0.451 (from R417888)	377	0.1	0.9
Imazamox*	active	305.3	-	16.7	11.6	0.936
CL 312622*	metabolite	305.3	0.829 (from as)	24.6	30.6	0.974
CL 354825	metabolite	277.3	0.778 (from CL 312622)	382	500	0.789
Azoxystrobin	active substance	403.4	-	78	423	0.86
CyPM	metabolite	398.4	0.874 (from as)	55.4	83	0.8
Flufenacet°	active substance	363.3	-	12.09	221.25	0.919
FOE Thiadone+	metabolite	170.1	0.570 (from as)	1.95	42.1	0.764
TFA§	metabolite	114	0.430 (from as) 0.531 (from FOE Thiadone)	1000	0.0001	1.0
Metazachlor	active substance	277.8	-	6.8	110	0.877
479M04	metabolite	273.3	0.1 (from as)	56.4	9.1	1.0
479M08	metabolite	323.4	0.112 (from as)	116.4	10	0.831
479M09	metabolite	349.4	0.06 (from as)	16.9	5.8	0.897
479M011	metabolite	305.4	0.143 (from as)	25.2	20.5	0.859

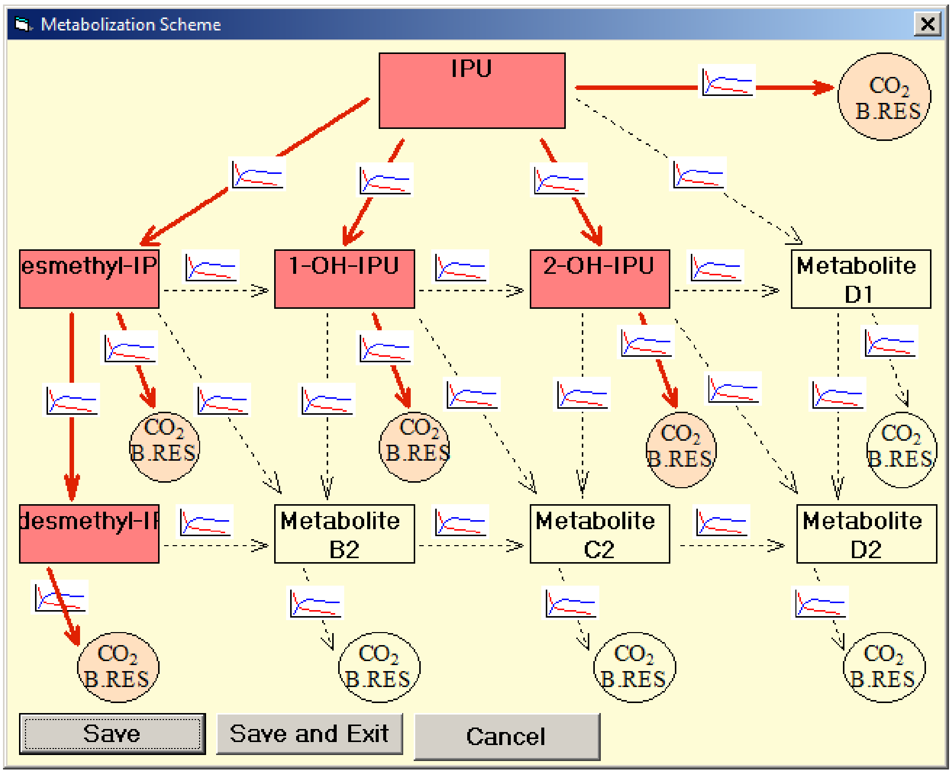
*: PUF=0.5 ° PUF=0.233 +: PUF = 0.452 §: PUF=0.0003.

Figure 119: **Metabolism scheme used to simulate the exposure of S-metolachlor and its soil metabolites with PELMO**



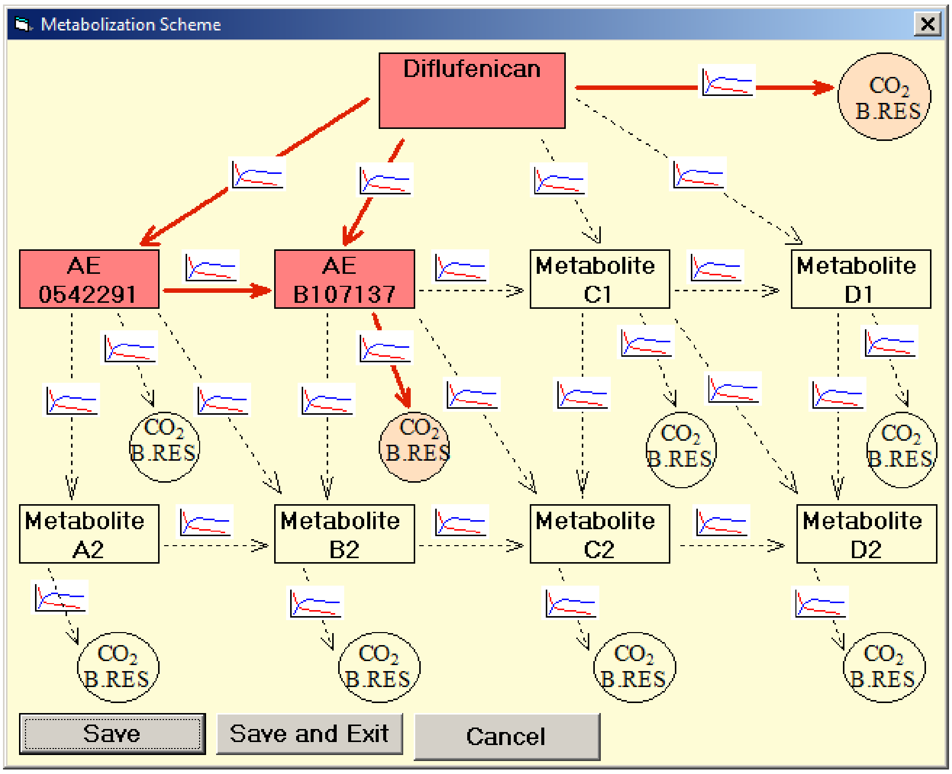
Source: own illustration, Fraunhofer IME.

Figure 120: **Metabolism scheme used to simulate the exposure of isoproturon and its soil metabolites with PELMO**



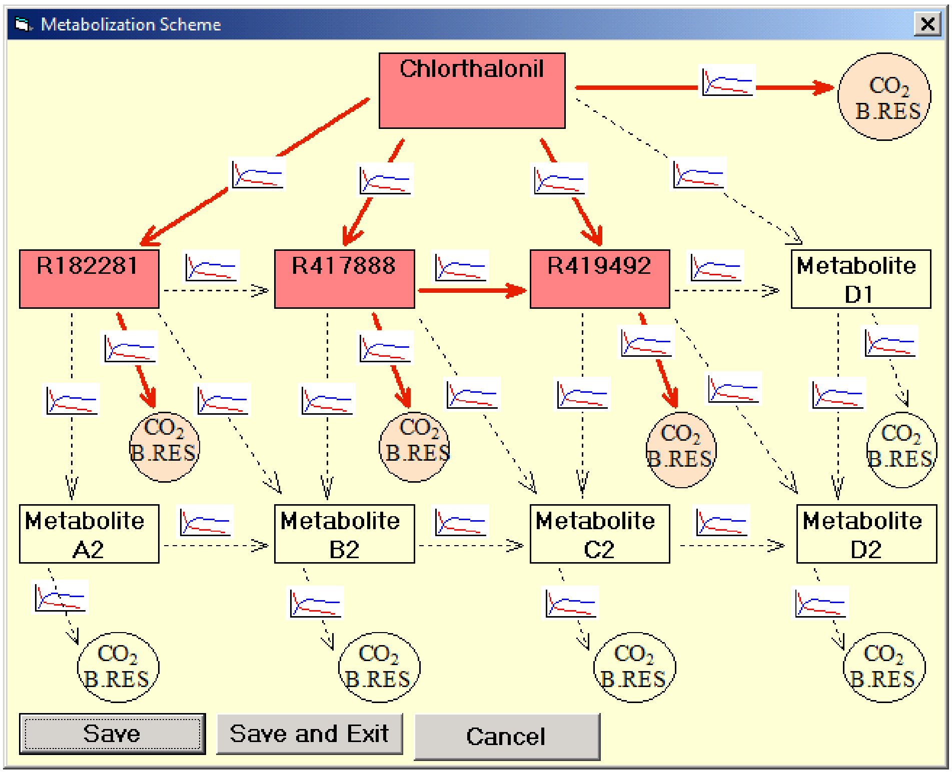
Source: own illustration, Fraunhofer IME.

Figure 121: Metabolism scheme used to simulate the exposure of diflufenican and its soil metabolites with PELMO



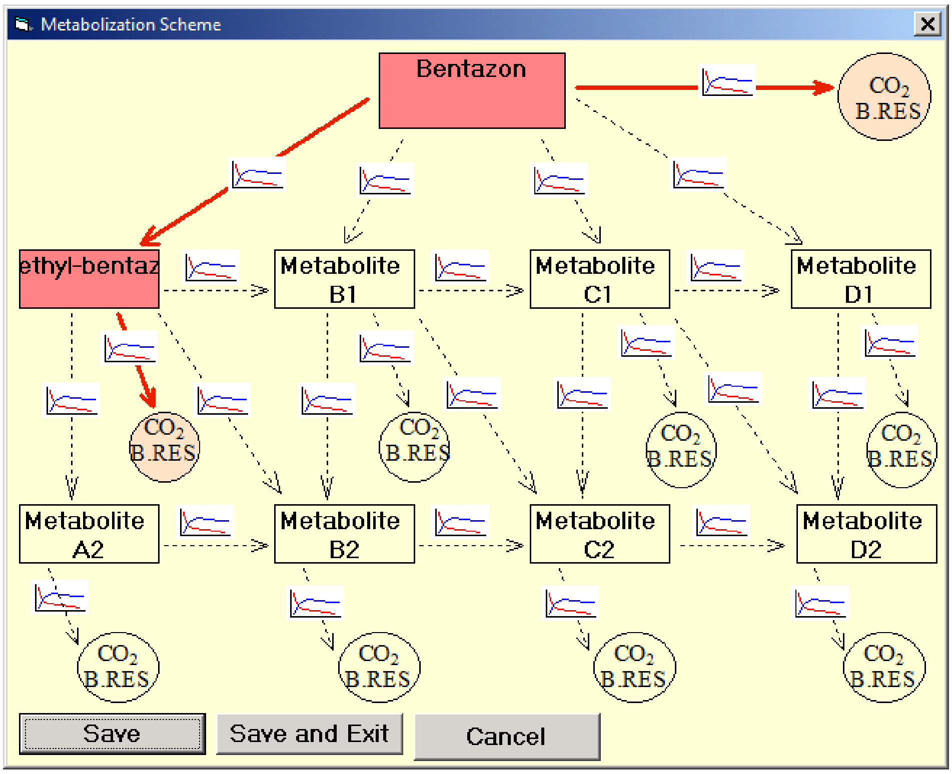
Source: own illustration, Fraunhofer IME.

Figure 122: Metabolism scheme used to simulate the exposure of chlorothalonil and its soil metabolites with PELMO



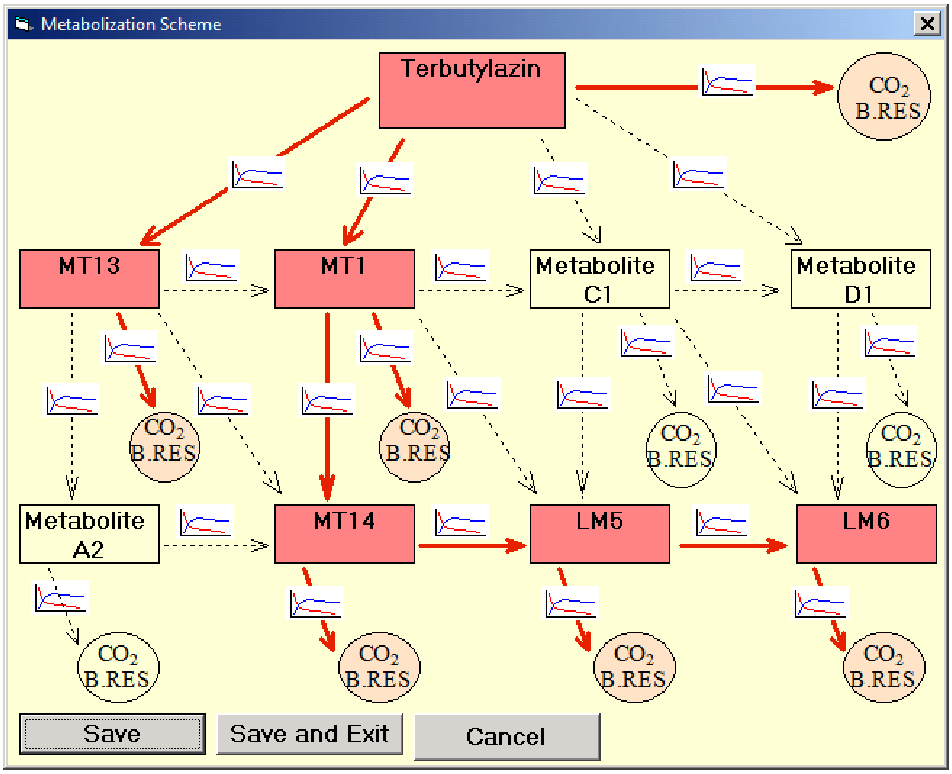
Source: own illustration, Fraunhofer IME.

Figure 123: **Metabolism scheme used to simulate the exposure of bentazone and its soil metabolites with PELMO**



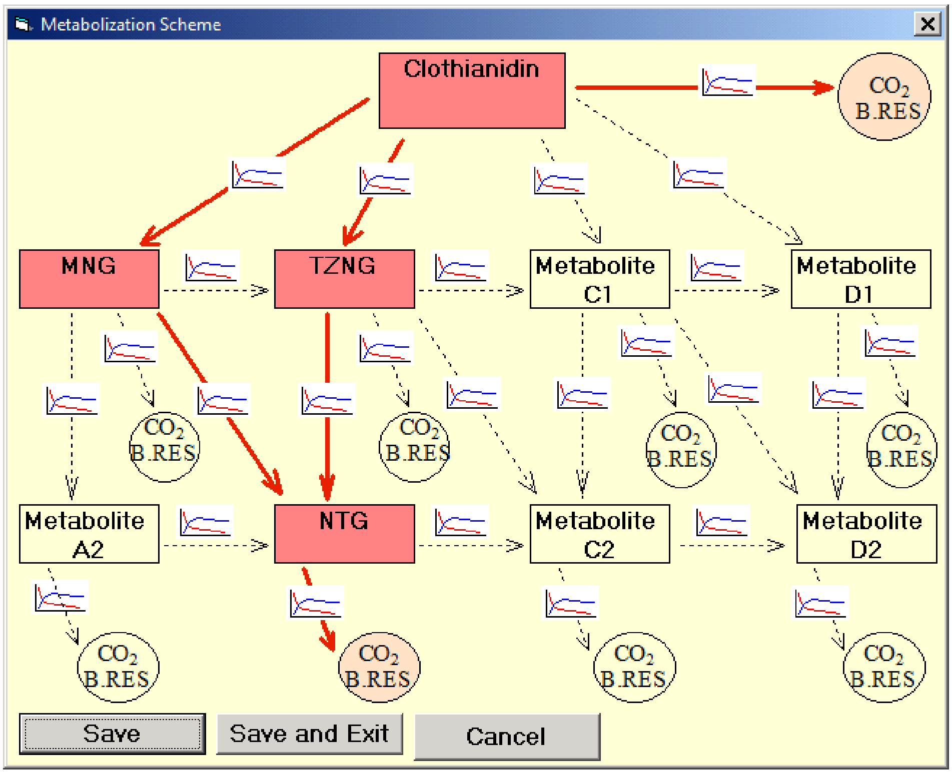
Source: own illustration, Fraunhofer IME.

Figure 124: **Metabolism scheme used to simulate the exposure of terbuthylazine and its soil metabolites with PELMO**



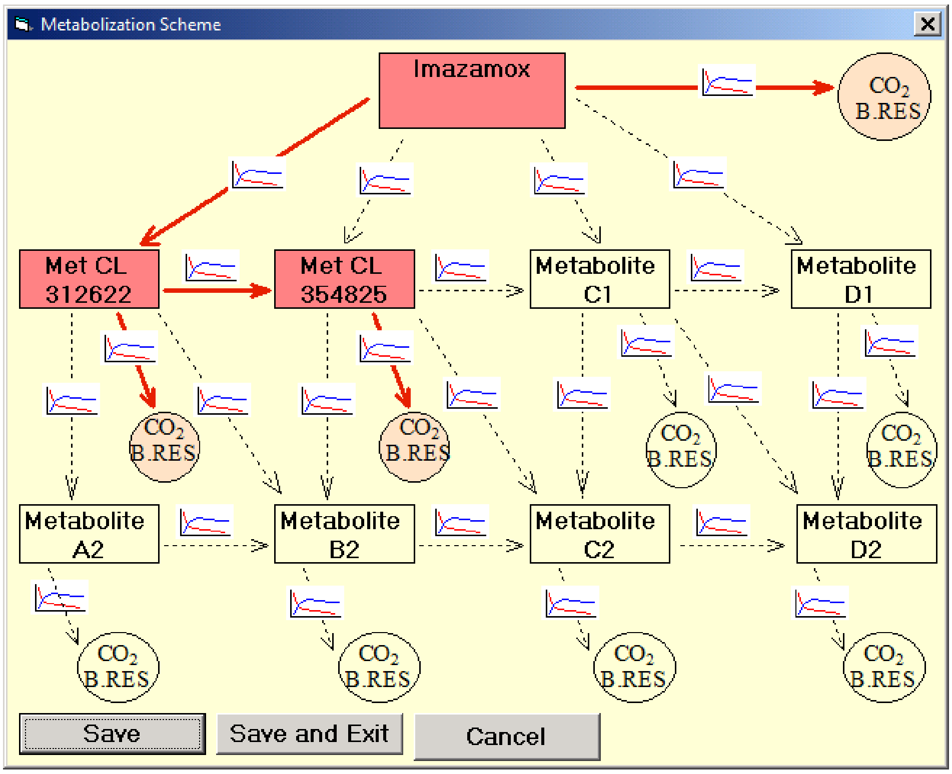
Source: own illustration, Fraunhofer IME.

Figure 125: Metabolism scheme used to simulate the exposure of clothianidin and its soil metabolites with PELMO



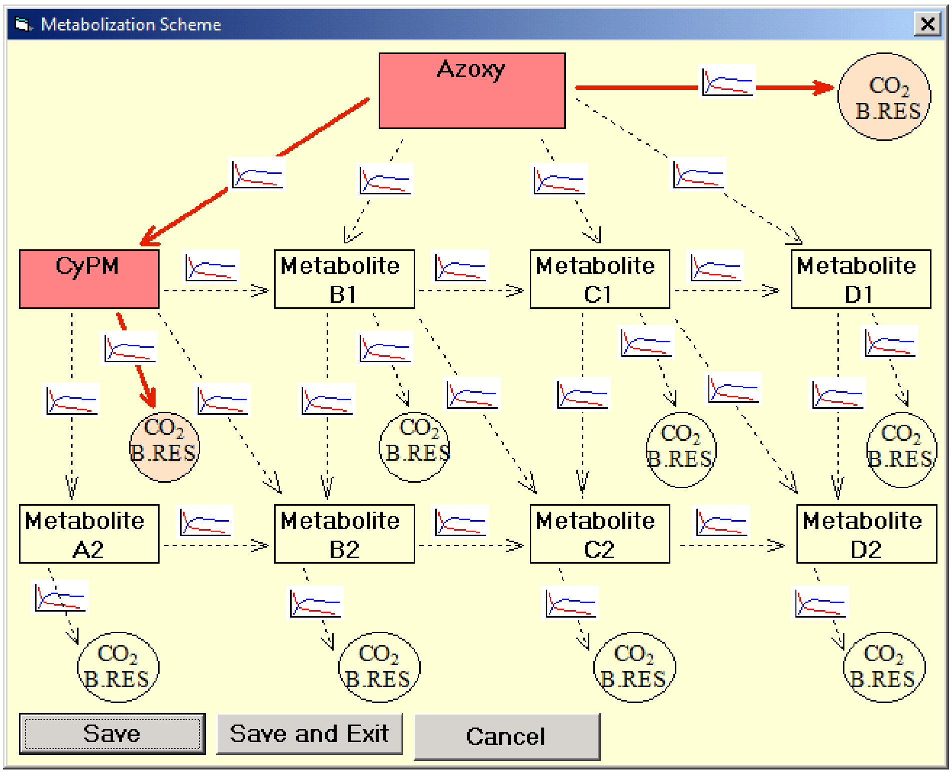
Source: own illustration, Fraunhofer IME.

Figure 126: Metabolism scheme used to simulate the exposure of imazamox and its soil metabolites with PELMO



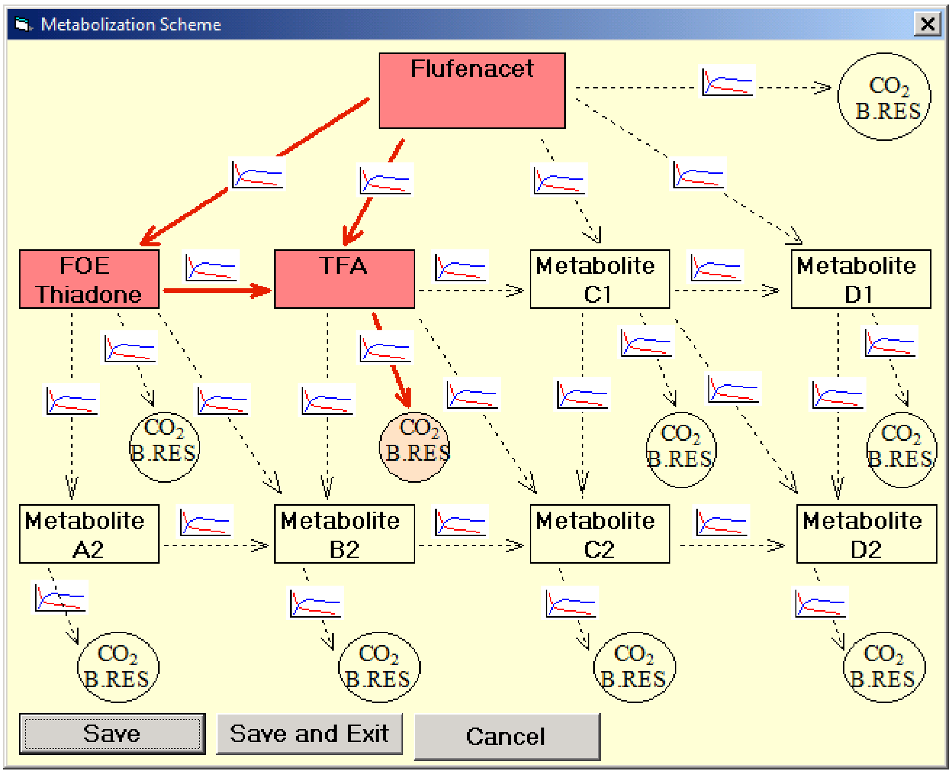
Source: own illustration, Fraunhofer IME.

Figure 127: **Metabolism scheme used to simulate the exposure of azoxystrobin and its soil metabolites with PELMO**



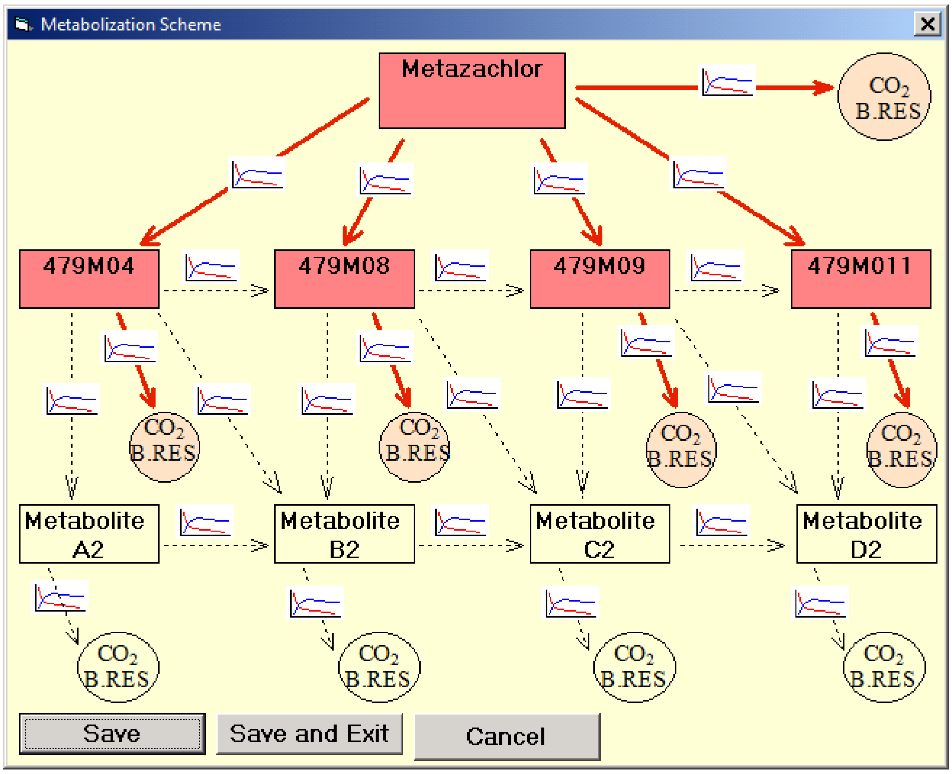
Source: own illustration, Fraunhofer IME.

Figure 128: **Metabolism scheme used to simulate the exposure of flufenacet and its soil metabolites with PELMO**



Source: own illustration, Fraunhofer IME.

Figure 129: Metabolism scheme used to simulate the exposure of metazachlor and its soil metabolites with PELMO



Source: own illustration, Fraunhofer IM