Xplicit – A Modelling Framework for Ecological Risk Characterisation at Landscape-scales in Regulatory Risk Assessment and Risk Management of Plant Protection Products

von

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"Ean woas hot doas fer e Bewandtnis?"

(Oberhessisch formulierte Frage welcher Sinn und Zweck einer Sache innewohnt)

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1 Terms and Definitions

General abbreviations used in this thesis are defined in Table 1. Likewise, basic terms are briefly described below. More specific terms and abbreviations are defined in corresponding sections.

Table 1: Abbreviations frequently used in this thesis.

Abbreviation	Definition
AE	Assessment Endpoint
AF	Assessment Factor
a.s.	Active substance (of a Plant Protection Product)
ATKIS	Authoritative Topographic-Cartographic Information System ('Amtliches Topographisch-Kartographisches Informationssystem')
BCS	Bayer CropScience
CPU	Central Processing Unit
eFate	Environmental fate (*e.g.*, of active substances)
EFSA	European Food Safety Authority
EP	Exposure-Path
ERA	Synonymously used for 'Environmental Risk Assessment' and 'Ecological Risk Assessment'
FAO	Food and Agriculture Organisation
FMEA	Failure Modes and Effects Analysis
GIS	Geographic Information System
GUID	Globally Unique Identifier
HTTP	Hypertext Transfer Protocol
ID	Identifier
IT	Information Technology
LM3	Landscape Metric (version 3)
LOD	Limit of detection
LULC	Land use / land cover
MC	Monte Carlo
NTA	Non-Target-Arthropod
NTTP	Non-Target-Terrestrial Plants
OOP	Object-Oriented-Programming
P()	Probability
PDF, PMF	Probability Density Function, Probability Mass Function
PEC	Predicted Environmental Concentration, *e.g.*, PECsw = PEC in surface water
PPM	Plant protection measure
PPP	Plant Protection Product

Abbreviation	Definition
QA	Quality Attributes
RA	Risk Assessment
RDBMS	Relational Database Management System
RM	Risk Management
RQ	Risk Quotient
SA	Sensitivity Analysis
SOA	Service-Oriented Architecture
SPG	Specific Protection Goal
SQL	Structured Query Language
SR	Study Region
TER	Toxicity Exposure Ratio
UA	Uncertainty Analysis
UASA	Uncertainty Analysis And Sensitivity Analysis
WB, WBs	Water body, water bodies
XA	Xplicit-Assess
XDist	Xplicit-Distance
XE	Xplicit-Engine
XF	Xplicit-Frontend
XM	Xplicit-Management
XML	Extensible Markup Language
XP	Xplicit-Processor
XSD	XML Schema Definition

Scales: This term is used in two ways; (i) mapping scale, where, *e.g.,* 1:5,000 represents a large scale and 1:250,000 a small scale; (ii) spatial or temporal unit, either defined numerically (*e.g.,* 10^0-10^1 m, 1 day), or represented by natural or conceptual objects (*e.g.,* 'region', 'receptor', 'WB segment'). The terms 'landscape-scale' and 'regional-scale' are used interchangeably only in relation to extent. A *region* refers to a spatial unit but the term *landscape* also represents an expression of human perception (Section 4.2). Experience in communication of landscape-scale risk characterisation has shown that, if not explicitly referring to map scales, misunderstandings are avoided by using the 'natural' perception of the terms 'small-' and 'large-scale', namely as small and large extent. Thus, *e.g.,* the 'smallest unit of analysis' represents the smallest discretised object in spatial (or temporal) extent, *i.e.*, the highest resolution of the analysis.

Regulatory Science: The context of applied scientific concepts and approaches with the goal to support regulatory decision-making (*e.g.*, authorisation of PPPs). "*Regulatory Science is the science of developing new tools, standards, and approaches to assess the safety, efficacy, quality, and performance of all FDA-regulated products.*" (FDA 2013).

2 Executive Summary

Chemical plant protection is an essential element in integrated pest management and hence, in current crop production. The use of Plant Protection Products (PPPs) potentially involves ecological *risk*. This risk has to be characterised, assessed and managed.

For the coming years, an increasing need for agricultural products is expected. At the same time, preserving our natural resources and biodiversity *per se* is of equally fundamental importance. The relationship of our economic success and cultural progress to protecting the environment has been made plain in the Ecosystem Service concept. These distinct 'services' provide the foundation for defining ecological protection goals (Specific Protection Goals, SPGs) which can serve in the development of methods for ecological risk characterisation, assessment and management.

Ecological risk management (RM) of PPPs is a comprehensive process that includes different aspects and levels. RM is an implicit part of tiered risk assessment (RA) schemes and scenarios, yet RM also explicitly occurs as risk mitigation measures. At higher decision levels, RM takes further risks, besides ecological risk, into account (*e.g.*, economic). Therefore, ecological risk characterisation can include RM (mitigation measures) and can be part of higher level RM decision-making in a broader Ecosystem Service context.

The aim of this thesis is to contribute to improved quantification of ecological risk as a basis for RA and RM. The initial general objective had been entitled as "*… to estimate the spatial and temporal extent of exposure and effects…"* and was found to be closely related to forthcoming SPGs with their defined 'Risk Dimensions'.

An initial exploration of the regulatory framework of ecological RA and RM of PPPs and their use, carried out in the present thesis, emphasised the value of risk characterisation at landscape-scale. The landscape-scale provides the necessary and sufficient *context*, including abiotic and biotic processes, their interaction at different scales, as well as human activities. In particular, spatially (and temporally) explicit landscape-scale risk characterisation and RA can provide a direct basis for PPP-specific or generic RM. However, refined risk characterisation at landscape-scale does not necessarily try to mimic real-world complexity. The required degree of realism (complexity) depends on the goals of a RA and RM tier.

With the aim to structure the developments of introducing more context in ecological risk characterisation, two categorical perspectives are discussed in this thesis. (i) *AutContext* takes the PPP use specific risk characterisation perspective and corresponds to current RA processes, while introducing real-world landscape factors driving risk. Lower-tier ecotoxicological data and exposure scenarios can serve as starting points. Refined landscape-scale factors can comprise parameters affecting exposure and effects (*e.g.*, crop-to-habitat distances, spray-drift or run-off filtering, habitat structure and quality). (ii) The *SynContext* takes an ecological entity-centric perspective of risk characterisation (*e.g.*, individual, population, community, biodiversity) by taking basically all relevant abiotic and biotic factors into account which affect the entity (*e.g.*, landscape management and dynamics, cultivation practice, land cover, PPP use(s), environmental and ecological conditions). In a PPP-specific risk characterisation, RA and RM, PPP-specific effects would be assessed against this 'full picture'. The question of whether a transition to *SynContext* would require a paradigm change in regulatory RA and RM needs further investigation. However, this perspective can be regarded as a prerequisite for future developments towards an explicit ecological risk characterisation component in higher level RM decision (*e.g.*, cost/benefit level) as well as to address higher level protection goals (*e.g.*, biodiversity).

From the general need for tiered landscape-scale context in risk characterisation, specific requirements relevant to a landscape-scale model were developed in the present thesis, guided by the key objective of improved ecological risk quantification. In principle, for an adverse effect (*Impact*) to happen requires a sensitive species and life stage to co-occur with a significant exposure extent in space and time. Therefore, the quantification of the *Probability* of an *Impact* occurring is the basic requirement of the model. In a landscape-scale context, this means assessing the spatiotemporal distribution of species sensitivity and their potential exposure to the chemical.

The core functionality of the model should reflect the main problem structures in ecological risk characterisation, RA and RM, with particular relationship to SPGs, while being adaptable to specific RA problems. This resulted in the development of a modelling framework (*Xplicit-Framework*), realised in the present thesis. The *Xplicit-Framework* provides the core functionality for spatiotemporally explicit and probabilistic risk characterisation, together with interfaces to external models and services which are linked to the framework using specific adaptors (*Associated-Models*, *e.g.*, exposure, eFate and effect models, or geodata services). From the *Xplicit-Framework*, and using *Associated-Models*, specific models are derived, adapted to RA problems (*Xplicit-Models*).

Xplicit-Models are capable of propagating variability (and uncertainty) of real-world agricultural and environmental conditions to exposure and effects using Monte Carlo methods and, hence, to introduce landscape-scale context to risk characterisation. Scale-dependencies play a key role in landscape-scale processes and were taken into account, *e.g.*, in defining and sampling Probability Density Functions (PDFs). Likewise, evaluation of model outcome for risk characterisation is done at ecologically meaningful scales.

Xplicit-Models can be designed to explicitly address risk dimensions of SPGs. Their definition depends on the RA problem and tier. Thus, the Xplicit approach allows for stepwise introduction of landscape-scale context (factors and processes), *e.g.,* starting at the definitions of current standard RA (lower-tier) levels and taking the *AutContext* view (*i.e.*, centring on a specific PPP use, while introducing real-world landscape factors driving risk). With its generic and modular design, the *Xplicit-Framework* can also be employed in a *SynContext* approach (*i.e.*, taking an ecological entity-centric perspective). As the predictive power of landscape-scale risk characterisation increases, it is possible that *Xplicit-Models* become part of an explicit Ecosystem Services-oriented RM (*e.g.,* cost/benefit level).

In the present thesis, the potential of the Xplicit approach was demonstrated by case studies showing how more realism (context) can be introduced stepwise to refine risk characterisation. The case studies include example RAs for Non-Target-Arthropods (NTAs), Non-Target-Terrestrial Plants (NTTPs) and aquatic species. The range of RA problems and the spatial extents of the landscapes illustrate the adaptability and scalability of the approach. Starting from lower-tier RA levels, and related to SPGs, the results show how improved landscape-scale context (*AutContext*) can significantly increase risk characterisation. The results are considered to provide an evidently supportive part for RA and RM decisions. For the given RA problems, the results of the studies indicate that exposure and effects are limited in different risk dimensions when taking more realism into account. As a first approximation, the difference to the lower-tier risk characterisation was about one order of magnitude.

The studies demonstrate the value of spatiotemporally explicit and probabilistic calculations to build a sufficient basis for RM decision-making at higher organisation levels (*e.g.,* populations) and scales. As an overarching principle, scale dependencies need to be taken into account in all aspects, from the characterisation of variability (and uncertainty) up to the evaluation of outcome (risk characterisation, RA) and the implementation of RM measures.

The propagation of input data uncertainty to model outcome and conclusions is perceived as a major concern. At landscape-scale, preliminary results suggest that local scale parameter uncertainty might be only partly propagated to ecologically relevant scale(s). This hypothesis is proposed to be further investigated using a nested Monte Carlo approach.

In particular, the case studies demonstrate the immediate value of landscape-scale risk characterisation to identify efficient RM measures, for both, PPP specific mitigation and generic RM. The case studies also include preliminary concepts on the development of scenarios for refined risk characterisation of PPPs in SPG context ('Reference Scenarios'). Beyond the focus on PPP uses, at a *SynContext* level, a landscape-scale model like Xplicit can contribute to the identification of strategies for risk balancing among different Ecosystem Services and ecological protection goals.

Future development towards improved realism (context) first requires improved definition of RA targets (*e.g.,* SPGs), and hence, model purposes. On this basis, the necessary predictive power of landscape-scale models can be defined. Improved predictiveness needs further development and implementation of model processes (*e.g.,* exposure, eFate and ecological processes). Geodata on land use/cover are generally available at small mapping scales or can be generated in high resolution (large mapping scales), whereas ecological data, *e.g.,* on species occurrence or habitat suitability need to be improved. Progress in refined risk characterisation should consider the dynamic interaction of "*what is possible and what is necessary*". To this end, iterative development processes can provide a methodological means. The new levels of complexity in risk characterisation, RA and RM require explicit consideration of approaches and skills in risk communication.

Decision-making includes the existence of alternatives. Landscape-scale models, like Xplicit, can assess the consequences of alternatives, and hence, can support decision-making in an uncertain environment. Improved explicit ecological (and economic) understanding of consequences of alternative human activities is a prerequisite to balance them alongside societal objectives. This work intends to contribute to a possibly next generation of integrated crop production.

3 General Introduction

3.1 Background

Cultivated landscapes have provisioning as well as cultural meaning to humans. As they cover large areas, they represent flora and fauna habitats of likewise fundamental importance. Cultivated landscapes are ecosystems of distinct human influence, shaped by agriculture and other land uses. Landscapes provide a range of *services*, a human perspective that has been made plain in the Ecosystem Service concept (UNEP 2013). Taking this perspective, today, sustainable food production and protection of natural resources (biotic and abiotic) have become similarly important. Maintenance of biodiversity has become an overarching topic. The co-existence of intensive agricultural production with rich and viable ecosystems is a key challenge to agriculture and land management, especially in respect to a growing human population (≈9 billion by 2050, UN 2011a). The simple solution - to mainly separate cultivation areas from natural reserves - might be reasonable in some cases, but for the majority of landscapes, this runs against human tradition and culture. Thus, regional and local co-existence is the target.

Chemical plant protection is an essential element in integrated pest management (FAO 2013a). The use of Plant Protection Products (PPPs) rarely comes without any effects on other organisms than the targeted pests, either indirectly (*e.g.,* reducing food sources) or directly by having toxic effects. Thus, the use of PPPs potentially involves an ecological *risk* which has to be characterised, assessed and managed. The first step, risk characterisation, requires a quantitative detailed analysis of potential ecological effects and their probability of occurrence under real-world conditions. The second step, risk assessment (RA), is a regulatory act which relates the described risk to ecological protection goals. The third step, risk management (RM), acts on various levels. It can solely focus on the ecological level, but it can also take a broader Ecosystem Service perspective to balance ecological and economic risk (cost-benefit). RM includes the implementation of appropriate risk mitigation measures. Obviously, RA and RM closely interact.

Decision-making includes the existence of alternatives. The risk involved in doing something is always assessed relative to the risk of not doing it. RM alternatives can mean alternative mitigation measures for an individual PPP, alternative PPPs, alternative plant protection measures, or alternative management of cultivated landscapes. In each case, risk characterisation builds the basis.

Current ecological RA procedures for PPPs focus on the identification of low risk cases yet are not designed to quantify risk extent for representative conditions ('Reference Scenarios', EFSA 2010a). The relationship between standard RA and the RM levels (above) is hardly transparent, *e.g.*, "*what does reduced dry weight of a plant test species measured under conservative exposure conditions mean to real-world plant communities, or even to Ecosystem Services?*". Present developments in regulatory science point towards improved characterisation of risk. With the introduction of Specific Protection Goals (EFSA 2010a, 2010b), quantification of risk in different dimensions is required (*e.g.*, biological entity, attribute, magnitude, space, time), based on more realistic context. This context can be derived at landscape-scale which is also the focal scale of RM. The present work is intended as a step towards a refined ecological risk characterisation and, thus, as a contribution to bridge the gap between current standard RA and requirements for broader real-world context in RA and RM.

3.2 Objectives

Experience in recent years using geodata in RA and RM of Plant Protection Products encouraged the examination of important aspects of landscape-scale exposure and effect modelling. Initial thoughts suggested the necessity for a spatiotemporally explicit and probabilistic approach with distinct consideration of scales (Schad 2006a). Scale dependencies should be taken into account in different aspects of risk characterisation, from the propagation of parameter variability (and uncertainty) in the model up to ecological risk characterisation.

The initial general objective had been entitled "*… to estimate the spatial and temporal extent of exposure and effects…", and* "*… to improve risk quantification for Non-Target-Organisms …*".

Half-way through this project, an opinion of the European Food Safety Agency (EFSA) on Specific Protection Goals (SPGs) was published (EFSA 2010a) and a related workshop was held (EFSA 2010b). In the EFSA opinion, protection goals are explicitly discussed in terms of *Risk Dimensions* and *Scales*, among which in particular, the spatial and the temporal scale are included. Key aspects discussed in the context of SPGs fitted well with the objectives of this thesis – generally spoken '*Landscape-scale RA and SPGs are linked*'. Risk characterisation in terms of *Risk Dimensions* requires methods and data for spatiotemporally explicit exposure and effect modelling.

In this thesis, the topic of landscape-scale risk characterisation was intended to be developed further in order to make a contribution to improve regulatory RA and RM of Plant Protection Products. Therefore, the general objective of this thesis was broken into consecutive targets:

1 Identification of requirements for landscape-scale exposure and effect modelling in regulatory RA and RM of Plant Protection Products. Transfer of requirements into *concepts* and a suitable *approach* for multidimensional risk characterisation.

2 Development of a computer model for ecological risk characterisation at landscape-scales based on the requirements derived at step (1), with particular attention to handle the complexity inherent to landscape-scale modelling. To this end, the model should allow for stepwise introduction of more realistic landscape-scale context into RA and RM and hence, to operate at different complexity levels.

3 Use and discussion of the model approach in example RA problems in context to SPGs.

3.3 Sections

According to the three key objectives (Section 3.2), the thesis contains three main sections (Figure 1):

- Part 1 (Section 4) explores the literature on the regulatory framework regarding RA and RM of PPPs and their use, the current RA and RM practice as well as developments in regulatory science. Landscape-scale context, relevant for risk characterisation, RA and RM, is reflected in a theoretical discourse. On this basis, general requirements for model approaches for exposure and effect assessment at landscape-scale are developed.
- Part 2 (Section 5) presents the development of a modelling framework ('Xplicit') for risk characterisation at landscape-scales, based on the outcome of Part 1. The development considers conceptual and technical aspects. Contemporary methods of software development are shown with particular emphasis on modularity. The section closes with the preparation of specific *Xplicit-Models* ready to be used in landscape-scale RA and RM.
- In Part 3 (Section 6), *Xplicit-Models* are exemplarily used in specific landscape-scale RA problems. Problem formulations, approaches and generic results are discussed and proposals for future developments are provided.

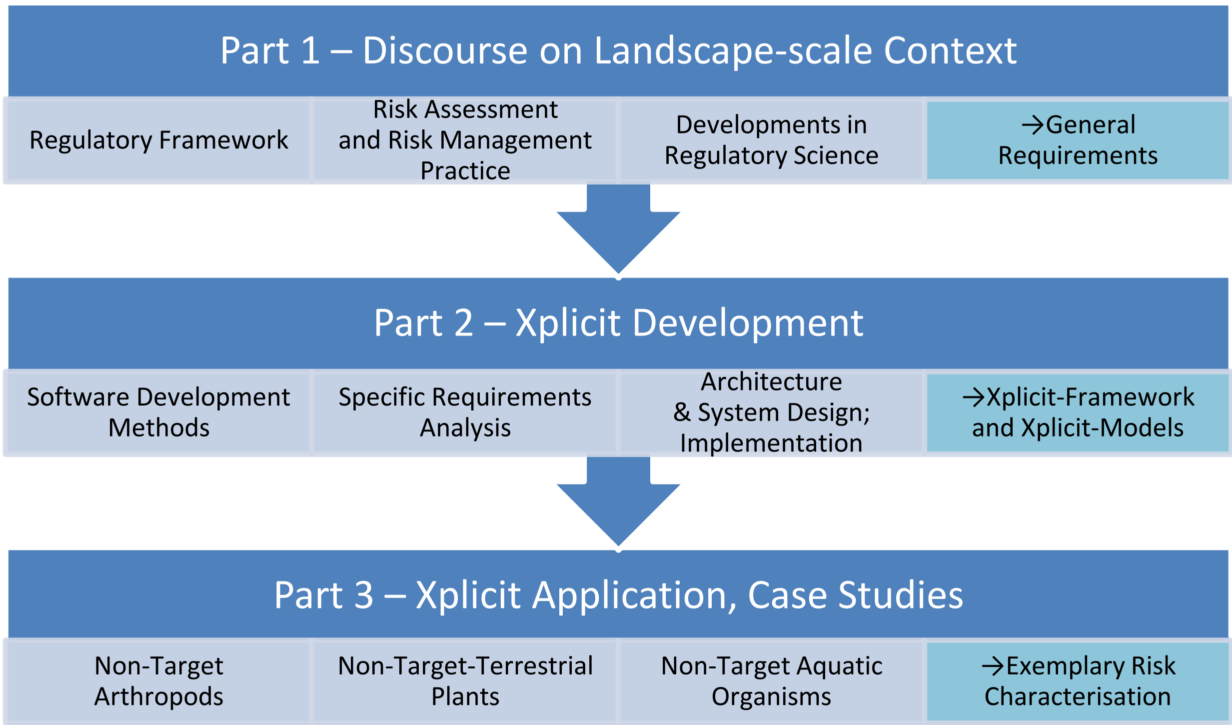


Figure 1: Main sections of this thesis with their major work topics and outcome ('→' in highlighted boxes).

3.4 Limits of Feasibility

The range of aspects touched upon in landscape-scale risk characterisation is very large. Disciplines involved range from regulatory RA procedures with underlying protection goals, RM, agricultural practices, exposure and environmental fate modelling, ecotoxicological effect assessment, ecological modelling, to numerous technical aspects of geodata processing or probabilistic methods, up to risk communication. This required focusing on essential aspects in order to achieve the objectives of this thesis given in Section 3.2.

The idea of the present work is to start at the current processes in regulatory RA (exposure and effect assessment) and RM as a basis to *stepwise* introduce more realistic risk driving factors, yet to design an approach which is able to deal with increasing levels of complexity. Current capabilities of *Xplicit-Models* and future options are reflected in the case studies (Section 6) and in the development Sections 5.4 and 5.5.

4 Part 1: Landscape Context in Regulatory Ecological Risk Assessment and Risk Management of Plant Protection Products

This section summarises an examination of the relevance of landscape-scale approaches in ecological RA and RM for PPPs. The evaluation was intended to be sufficiently comprehensive to lay the foundation for the development of a landscape-scale model and its implementation ('Part 2', Section 5).

4.1 Summary

Ecological RA of PPPs generally follows tiered assessment schemes (*e.g.*, FOCUS 2001, EC 2002a, 2002b, EFSA 2009, 2012b). Standard RA scenarios (lower-tier, 'Tier-1') basically use a Toxicity Exposure Ratio (TER) which effectively relates low ecotoxicological endpoints to high exposure values, both values representing relative extremes of expected real-world variability. Additional 'Assessment Factors' (AFs) are imposed to account for uncertainties (mainly in species sensitivity). As to their protective intention and targeting at the edge-of-the-field scale, lower-tier assessment scenarios have an implicit risk definition, *i.e.*, real-world risk extent is not explicitly quantified.

With the implementation of SPGs (EFSA 2010a, Section 4.3.2.1), risk characterisation of PPPs will have to cover multiple dimensions including amongst others explicit quantification of spatial and temporal risk extents, taking ecologically relevant scales into account. Further regulatory requirements and development goals (Section 4.3.2, 4.3.3) which also directly or indirectly refer to the authorisation and use of PPPs will require more explicit risk characterisation, RA and RM. In their entirety, current and forthcoming regulatory requirements reflect the range of Ecosystem Services (Millennium Ecosystem Assessment 2005). This background suggests the need for correspondingly adapted concepts and approaches in risk characterisation, RA and RM of PPPs.

Cultivated landscapes are basically anthropogenic. Land use, management and its dynamics largely affect species occurrence, abundance and population dynamics. The landscape-scale can be regarded as an integrative unit providing the necessary and sufficient context to ecological risk characterisation in regulatory RA and RM of PPPs with respect to abiotic and biotic factors, processes, and their interaction ("*Landscape = Context*"). Different context levels can be employed in PPP-specific RAs to refine risk characterisation (Section 4.2, Figure 3), as well as in generic development efforts, *e.g.*, in the development of ecological scenarios (Reference Scenarios, EFSA 2010a). Context levels can also support stepwise approaches towards refined risk characterisation to ensure consistency with existing RA and RM procedures and traceability of outcome and conclusions.

The definition of risk, as employed in this thesis and commonly used in RA of PPPs, incorporates a well-defined adverse effect (*Impact*) and the related probability that this effect occurs. At individual level, an adverse effect to happen requires a sensitive species and life stage to co-occur with a significant exposure extent in space and time. These spatiotemporal coordinates (r,t) provide a first indication of the spatiotemporal variability of ecological risk due to PPP use, and its direct relationship to the landscape-scale. Therefore, and with respect to developments in regulations and regulatory science, a next generation of landscape-scale concepts and approaches in risk characterisation is proposed.

Concepts should be consistent for RA problems of structural similarity. This leads to a sufficiently generic approach which is adaptable to RA problems in a SPGs context. Options for stepwise introduction of context and complexity in risk characterisation are regarded as necessary to keep the relationship to current RA procedures and to assure traceability of results ('*from protective to predictive*'). This applies to higher-tier approaches as well as to scenario development for future tiered RA schemes. Spatially and temporally explicit risk characterisation at relevant landscape-scales on the basis of more realistic (real-world) conditions is regarded as a necessary basis for refined RA and effective RM.

Besides spatiotemporally explicitness and the use of geodata, the landscape-scale model should consider a probabilistic approach as a means to propagate variability (and uncertainty) of landscape factors to variability of risk as well as the explicit consideration of scales at all processing steps (risk characterisation, RA and RM). The model should be adaptable to a range of typical ecological RA problems of PPPs. A modular implementation is preferred in order to manage the inherent complexity of landscape-scale approaches.

With their explicit characterisation of risk, the steadily increasing predictive power of landscape-scale models can cause new regulatory challenges, *e.g.,* a demand for statements on explicit real-word risk acceptance and RM.

4.2 Cultivated Landscapes as a Context-Providing Unit in Risk Characterisation

Cultivated landscapes are closely related to human activities. For a childhood on a farm (Figure 2), the surrounding landscape was a direct part of life. It was 'nature', playground and production area, the immediate basis of life - "*a symbiosis of culture and nature*". In 1970ies, although changes from traditional livelihood of agriculture to other trades were in full progress, the majority of farms were still in operation. The diversity of land use, composing of arable fields, meadows, orchards, forest, etc. (Figure 2), and the landscape structure reflected the farming in the village and their product diversity (dairy farming, pigs, cattle, eggs, fruit, cereals).

Within a generation, the situation of *agriculture* substantially changed. Today, a single farmer has remained making a living solely on agriculture. This development was accompanied by changes in land use and structure. For a period, farmers who stopped dairy farming but had their machinery left for arable cultivation and harvesting, turned meadows into arable land. With the decrease of this 'side-line income' meadows were reintroduced, *e.g.*, for horses (hobby). In the same period, commodity prices, land consolidation and regulations (*e.g.*, European regulation on set-asides, EWG 1992) affected field types and sizes, rural roads, as well as land cover types like hedges, groves, orchards meadows, streams, and fallow land. Nature conservation projects supported semi-natural grassland (*e.g.*, using sheep flocks) or orchards.

This brief history illustrates that cultivated landscapes are highly dynamic. Dynamics occur in at different landscape-scales, ranging from local patches to large regions in spatial scales, and across a large range of temporal scales (here, some decades). Characteristics of cultivated land-scapes are driven by anthropogenic management, guided by the societal objectives of their time.

Figure 2: Core of a village in Hessian end of the 20th century (left) and surrounding cultivated landscape (right) (with the kind permission of D Cuda).

Biodiversity in cultivated landscapes is largely related to land use/cover, landscape structure and dynamics (Leitao *et al.* 2006, BMELV 2005, Ellis & Pontius 2013, Levin 1998). Thus, land management is a key factor of species occurrence, abundance and population dynamics. Land management can be an advantage for species A and a disadvantage for a species B. The relationship of human activities to cultivated landscape characteristics and biodiversity shows that there is rarely a *per se* (self-evident) biodiversity status, but societal objectives comprising economic and ecological goals.

Beyond material factors, cultivated landscapes have a spiritual meaning to humans. "*Daniels & Cosgrove defined landscape, not in physical terms but as an outward expression of human perception: a landscape is a cultural image, a pictorial way of representing, structuring or symbolising surroundings."* (wikipedia.org, Cosgrove & Daniels 1988).

The range of values of natural resources and processes to humans is quantified in the Ecosystem Services approach (Millennium Ecosystem Assessment 2005). The concepts build a key role in the definition of Specific Protection Goals (EFSA 2010a, Section 4.3) as a basis and framework for regulatory ecological RA and RM of PPPs.

This background allows to consider the landscape-scale as the unit providing the necessary and sufficient context for ecological risk characterisation in regulatory RA and RM of PPPs with respect to abiotic and biotic factors, processes, and their interaction ("*Landscape = Context*"). This context is complex by nature. Therefore, categorical context levels are proposed to provide some orientation in landscape-scale risk characterisation (Figure 3). These context levels can be employed in PPP-specific studies to refine risk characterisation as well as in generic development efforts, *e.g.*, in the development of ecological scenarios (Reference Scenarios, EFSA 2010a). The context levels can also support stepwise approaches to ensure consistency with existing RA and RM procedures and traceability of outcome and conclusions.

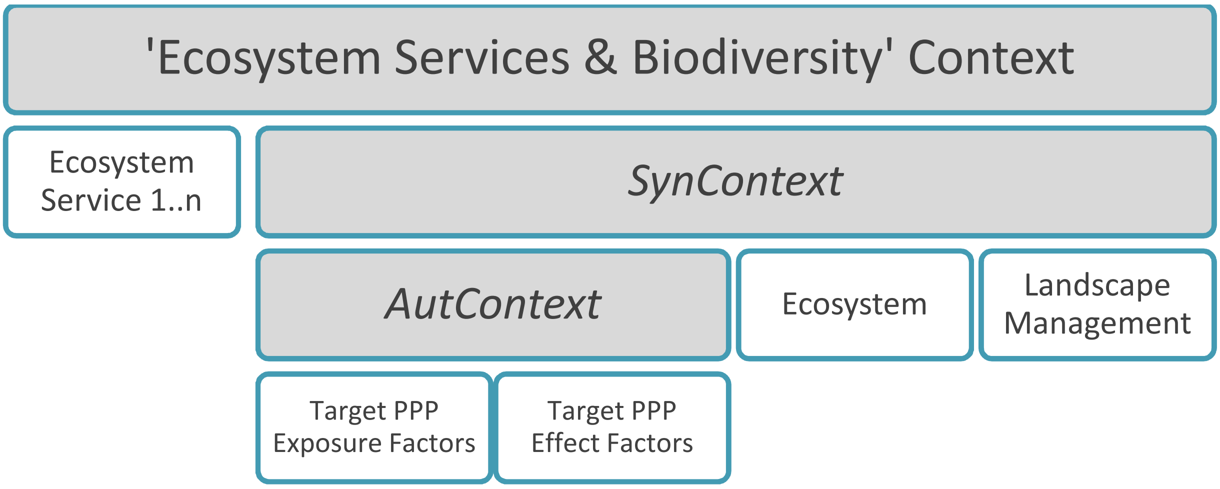


Figure 3: Simple scheme on categorical context levels in landscape-scale risk characterisation, RA and RM (*AutContext*, *SynContext*, 'Ecosystem Services & Biodiversity' context; grey boxes) and their major context-building blocks. ('Ecosystem Service 1..n' includes services of immediate economic value, *e.g.*, food production; detailed explanations on the context levels are provided in this section).

- *AutContext*: PPP specific risk characterisation perspective focusing on the 'target PPP' which is subject of the RA. This context level corresponds to the design of current RA processes (Section 4.3.2) but introduces real-world landscape factors which are immediate drivers of risk. Lower-tier ecotoxicological data and exposure scenarios can serve as starting points and can provide conservative scenario definitions. Refined landscape-scale factors can comprise parameters affecting exposure (*e.g.*, crop-to-habitat distances, spray-drift or run-off filtering, dissipation) or transfer of individual level effects to (meta-) population and community level of a sensitive species or trait. The occurrence of lower-tier scenario assumptions can be set in context to real-world conditions.
- *SynContext*: Ecological entity(ies) centric risk characterisation perspective (*e.g.*, individual, population, community, biodiversity). Characterisation of the entity(ies) taking all relevant abiotic and biotic factors into account (*e.g.*, 'ecosystem', landscape management, cultivation practice, land use, PPP uses, environmental conditions, dynamics). A PPP-specific risk characterisation, RA and RM are assessed against this 'full picture'.
- 'Ecosystem Services & Biodiversity': Ecosystem Services and biodiversity perspective, considering ecological and economic risk. At this level, the landscape-scale approach is based on all relevant data and processes to provide a means to assess ecological and economic consequences of an action as a basis for higher level RM decisions (*e.g.*, benefit of a PPP measure against ecological risk). This represents the necessary context level to address the "*food & biodiversity*" problem, *i.e.*, to identify strategies for sustainable food production and biodiversity goals.

This first attempt to structure context levels emphasises the relevance of the landscape-scale perspective in risk characterisation, RA and RM, and provides a first idea on how relevant context can be implemented into risk characterisation according to studies objectives.

4.3 Principles, Policies and Regulations in Ecological Risk Assessment and Risk Management of Plant Protection Products

"*Pesticide policy aims to minimise the risks without losing the benefits.*" (Department for Environment, Food and Rural Affairs, DEFRA, UK)

This section summarises aspects of the regulatory framework directly or indirectly referring to the authorisation of chemicals as Plant Protection Products in Europe and its Member States with respect to potential ecological risk. The evaluation aims at a characterisation of regulatory requirements regarding ecological RA and RM with respect to landscape-scale risk characterisation approaches.

4.3.1 Risk – Assessment, Management and Communication

4.3.1.1 Risk

Prior to conducting a risk characterisation, the term *risk* needs to be defined in order to provide an unambiguous basis for RA and RM decision-making. First of all, *risk* includes a choice of taking an action or not. With respect to risk of a PPP, this can comprise, *e.g.*, the authorisation of its intended use, or the imposition of risk mitigation measures on its use, or not authorising its use. Practical usage of the term *risk* is ambiguous. Often the term *risk* is used for the possibility (chance) of an adverse effect occurring: *e.g.* "*risk that population abundance is significantly reduced is 50%*", whereas "chance" is what is actually meant ("*the chance (or possibility) that population …*").

Basically, *risk* describes the *result* of an uncertainty on a specified phenomenon to happen (Bedford & Cooke 2001). Thus, *risk* incorporates (i) a well-defined adverse effect extent (*Impact*), and (ii) the *Probability* that this *Impact* occurs (Equation 1):

Risk = Impact x Probability (Equation 1)

Impact: potential extent of an adverse effect, potential loss/damage/hazard/incident.

Probability: likelihood (chance) that the *Impact* occurs.

The *Impact* can be further broken down by, *e.g.*, separating the incident from its consequences (*e.g.*, incident: plane crash; consequence: number of causalities). In ecological risk characterisation, the *Impact* is characterised by the Assessment Endpoint (consisting of the biological entity and the assessed attribute) and the effect extent. Assessment Endpoints are determined in relation to protection goals (Section 4.3.2), and hence, need to represent ecologically relevant *Impact* descriptors which are accessible to prediction and monitoring (Suter 1990). Biological entities of Assessment Endpoints can range from individual level (*e.g.*, endangered species) to (meta-) population, communities or biodiversity as such. Typical attributes of Assessment Endpoints are, *e.g.*, mortality, growth inhibition, clutch size reduction, reduction of population abundance, time-to-recovery, *etc.* (EFSA 2010a, 2010b).

Two major interpretations of *Probability* are commonly distinguished: (i) the frequentist view (empirical), and (ii) the subjectivist view (Bayesian view) (Cullen & Frey 1999, Morgan & Herion 2007). The frequentist takes the value as *Probability* to which the long-run frequency (the number of events in a sequence of trials) converges as the number of trials increases. This approach to estimate *Probability* is taken by the *Xplicit-Framework* (Part 2, Section 5). In the subjectivist view, the *Probability* of an event is estimated based on evidence, *i.e.*, based on available information. Thus, the *Probability* depends not only on the event, but represents a state of knowledge.

Dealing with uncertainty at different levels of ecological RA and RM (*e.g.*, complex higher-tier studies, definition of protection goals, definition of tiered assessment schemes and their scenarios) inevitably employs the Bayesian view as a range of data and risk characterisations (*e.g.*, including risk characterisation using Xplicit) have to be assessed on the background of personal experience of decision makers.

4.3.1.2 Risk Characterisation and Risk Assessment

In regulatory RA, the term 'Risk Assessment' is commonly used ambiguously: (i) the process of quantifying risk, and (ii) for the actual assessment of risk acceptability on the background of protection goals.

In this thesis, (i) is referred to as *risk characterisation*, representing the process of quantifying risk as defined above, including species exposure and effect extents as well as their *Probability* to occur. It comprises also a characterisation of assessment scales and dimensions of risk extents (Section 4.3.2.1). *e.g.*, "*at regional scale, there is a 5% chance of TER < 5 in more than 8% of the habitats due to spray-drift exposure*".

An adverse effect (*Impact*) to occur requires that (sensitive) organisms and the chemical co-occur in space and time. Thus, the quantification of the *Probability* of an *Impact* occurring requires the estimation of the spatiotemporal distribution of species sensitivity and their potential exposure to the chemical. *Probability* estimation can be derived from frequencies (Section 4.3.1.1) which are calculated on the basis of past experience (*e.g.*, long-term weather data, cultivation practice) without anticipation of future conditions. *Probabilities* in ecological risk characterisation typically range within some percentages (*e.g.*, ”*<10% chance to violate a trigger criteria*”), compared to, *e.g.*, catastrophic incidents with *Impact* to human life, like plane crashes or nuclear power station core meltdown, where very low probabilities are to be estimated.

According to the choice inherent in the term *risk*, the process of RA ((ii) above) compares the binary opportunities of whether risk resulting from the use of a PPP (possibly including mitigation measures) is acceptable or not. The relationship between risk characterisation and assessment of risk acceptability (RA) is illustrated in exemplary risk graphs in Figure 4.

The development of concepts and of a model approach for landscape-scale risk characterisation as a basis for regulatory RA and RM builds the key objective of this thesis (Section 3.2).

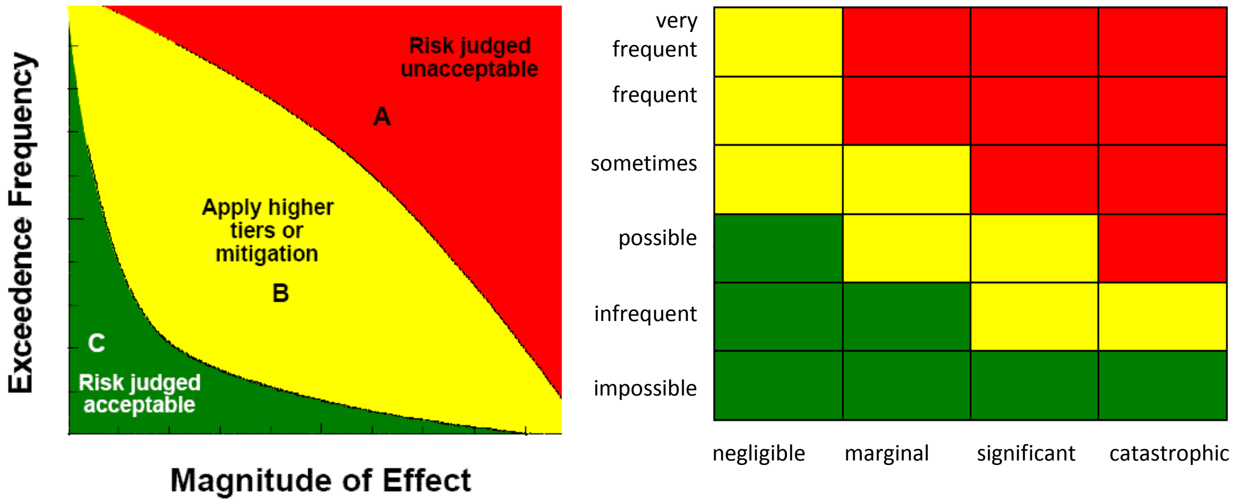


Figure 4: Continuous (left) and discrete (right) risk graphs. Example zones of 'acceptable' (green), 'unacceptable' (red) and 'ALARP' risk extent (yellow, 'As Low As Reasonably Practicable')(US EPA 2012).

4.3.1.3 Risk Management

The term risk management (RM) represents different levels of managing risk in order to avoid unacceptable risk. RM is part of risk characterisation and RA process in terms of mitigation measures (below). Ultimately, in the authorisation of PPPs, RM comprises the official act of balancing cost and benefits (ecological and economic risk). On European level, RA is done by the European Food Safety Authority (EFSA), and RM is done by the EU Commission (Directorate General for Health & Consumer, DG SANCO).

Risk mitigation comprises all measures and conditions that mitigate risk compared with the standard use situation considered during RA in accordance with the Uniform Principles (FOCUS 2007a, 2007b). Measures for active mitigation include, *e.g.*, application restrictions, use of spray-drift reducing application technology, no-spray (buffer zones), wind breaks, and vegetated filter strips. Passive mitigation refers to the absence of a vulnerable situation, *e.g.*, a shallow and unprotected water body (WB) close and downwind from a sprayed field. A review of mitigation measures considered by Member States and a collation of approaches available in the scientific literature for mitigating the exposure of surface water was conducted by the FOCUS Landscape & Mitigation group (FOCUS 2007a, 2007b).

Results of landscape-scale risk characterisation, as intended in this thesis, are considered to directly relate to RM. This includes PPP-specific risk mitigation measures and generic RM measures (*e.g.*, general buffer strip between fields and water bodies, constructed wetlands, Schulz *et al.* 2007, 2009, Stehle *et al.* 2011, Section 4.3.2.2).

4.3.1.4 Risk Communication

RM of PPPs comprises a broad range of disciplines, experts from different backgrounds and regulatory decision makers. The most sophisticated risk characterisation can be of limited use unless risk assessors and managers have confidence in it. Refined (higher-tier) risk characterisation studies obviously go beyond current detailed guidance. Yet, as long as done within a framework of general recommendations and leading opinions (*e.g.*, EC 2002a, 2002b, FOCUS 2007a, 2007b, EFSA 2010a, EFSA 2012b) the lack of detailed guidance should not form an obstacle to their acceptance in regulatory RA and RM. Improper risk communication, however, can form an obstacle. Thus, adequate communication of risk at all levels of risk characterisation, RA and RM is crucial to achieve ecological protection goals and economic objectives. With the introduction of SPGs (EFSA 2010a, Section 4.3.2) and their multidimensional risk characterisation, the challenge for risk communication will further increase.

Aspects of risk communication are implicitly included in risk characterisation, RA and RM procedures, *e.g.*, in reports of the FOCUS working groups (2001, 2007a, 2007b), EUFRAM (Hart 2006), Guidance Document on Aquatic Ecotoxicology (EC 2002a, EFSA 2012b). A key agreement that has been settled in ecological RA is in the interpretation of location parameters, *e.g.*, from distributions on exposure: *Typical Case* = 50th percentile (1-in-2), *Reasonable Worst Case* = 90th Percentile (1-in-10), and *Extreme Worst Case* = 99th Percentile (1-in-100) (SETAC, in CropLife International 1999). More recently, the importance of risk communication concepts and tools was recognised by EFSA (2010a) in its opinion on SPGs, which were intended to also support the dialogue between risk managers and risk assessors (specifically in the revision of the Ecotoxicology Guidance Documents, see below).

The general field of risk communication is well developed and is considered in a range of fields (*e.g.*, Lundgren & McMakin 2009). Also, general guidance on risk communication for chemicals is available (OECD 2002). However, in ecological risk characterisation, RA and RM of PPPs, risk communication has not yet become a discipline of comparable awareness and importance as the scientific tools. "*The lack of training of scientists in the field of risk communication may be one of the reasons why risk communication is not always as efficient as it should be*" (Streissel & Montforts 2010). With respect to future options of detailed ecological risk characterisations, training and tools for improved risk communication are needed (*e.g.*, Yau 2011, Steele & Lliinsky 2010). Competences from other disciplines such as communication, psychology, ethics, and design can support the development (Lundgren & McMakin 2009).

With their inherent complexity, risk characterisation, RA and RM at landscape-scale, immediately encounter problems of risk communication. In this thesis, attempts are made to aggregate multidimensional outcome of simulations in the context of SPGs (EFSA 2010a) and of the specific problem formulation. The presentation of results addresses the audience of experienced risk assessors (Part 3, Section 6).

4.3.2 Regulatory Framework

In the European Union (EU), the use of PPPs is regulated (European Food Safety Authority, EFSA 2013). EC Regulation 1107/2009 (EC 2009a) concerning the placing of PPPs on the market formulates general approval criteria for active substances, *e.g.*, "*it shall have no unacceptable effects on the environment, having particular regard to the following considerations where the scientific methods accepted by the Authority to assess such effects are available: … (i) its fate and distribution in the environment, … (ii) its impact on non-target species, … (iii) its impact on biodiversity and the ecosystem.*"

PPPs containing approved active substances are authorised by Member States (subsequent to adding the active substance to the positive list of approved active substances, *i.e.*, 'inclusion of the active substance in Annex I'). Three zones have been defined across Europe, in each of which authorities should share and mutually recognise PPP assessments (EC 2011). A risk envelop approach in a core assessment is considered to support harmonisation and to reduce efforts by focusing RA to uses representing the worst-case situation in each area of assessment (compartment). However, in cases where a Member State clearly identified specific national assessment requirements (differing from or extending the core assessment) which are necessary due to its specific environmental or agricultural circumstances, a national addendum is necessary (EC 2011), *i.e.*, effectively a RA according to national requirements. For example, German legislation (PflSchG 2010, BMELV 2012) targets at the *ecosystem* ('Naturhaushalt') in its general protection goals. RA of PPPs, including mitigation measures, is done by the Federal Environment Agency (UBA). The UBA also actively contributes to the development of national RA and RM criteria and approaches (*e.g.*, GeoRISK project, UBA 2010).

Awareness of the regulatory framework of ecological RA and RM at EU and Member State level as well as practices in regulatory decision-making processes is crucial to the development of landscape-scale approaches in regulatory science.

4.3.2.1 Specific Protection Goals

Regulatory RA and RM decision-making for PPPs need clear criteria regarding risk acceptability and risk characterisation procedures. General protection goals at EU (EC 2009a, *e.g.*, '*no decrease in biodiversity*') and national level need further specification.

As of this writing, Specific Protection Goals (SPGs) are under development ("*Risk assessors need to know what to protect, where to protect it and over what time period*.", EFSA 2010a, 2010b). Using the Ecosystem Service concept (*e.g.*, UNEP 2013), SPGs are considered for seven key drivers (microbes, algae, non-target plants (aquatic and terrestrial), aquatic invertebrates, terrestrial non target arthropods including honeybees, terrestrial non-arthropod invertebrates, and vertebrates), covering all ecosystem services which could potentially be affected by the use of PPPs (EFSA 2010a). The concepts are intended by EFSA as input for the dialogue between risk managers and risk assessors during the next steps of the revision of the Ecotoxicology Guidance Documents on Aquatic and Terrestrial Ecotoxicology (EC 2002a, 2002b, EFSA 2012b).

SPGs are anticipated to define risk dimensions (EFSA 2010a): "… *This requires specifying the following 6 dimensions or aspects of a specific protection goal: the ecological entity that is to be protected (individuals, (meta)populations, functional groups or ecosystems), the attribute(s) or* *characteristic(s) of that entity that must be protected (behaviour, survival/growth, abundance/biomass, processes, biodiversity), the magnitude of effect that can be tolerated for the attributes to be measured (biological scale), the temporal scale of effect (e.g. the maximum time on an annual basis over which single or repeated exposure/effect events are expected to exceed the critical level that can be tolerated), the spatial scale of the effect (e.g. the distance from the sites of application where the exposures and critical effect level to be tolerated are expected to occur), and the degree of certainty that the specified level of effect will not be exceeded. These dimensions are interdependent, and when considering the spatio-temporal dimensions of risk it is important to consider both exposure and effects and their spatio-temporal dimensions.*"

For the objectives of this thesis, the following aspects were extracted as of particular relevance:

- Multidimensional risk characterisation.
- The (meta-) population/community level represents a key *Biological Entity*.
- The occurrence of species and their abundance (resp. 'biodiversity') are key *Attributes*.
- Key *Biological Entities* and *Attributes* require an assessment of potential impacts at landscape-scale context (and beyond).
- Protection *Spatial Scales* range from edge-of-the-field to landscape.
- *Temporal Scales* of effects are to be assessed at periods ranging from days to years.
- Linking of exposure and effect assessments in terms of spatial and temporal scales.
- Importance of ecological scenarios development ('Reference Scenarios').
- Importance of a tiered approach for risk characterisation and RA. This is required to be appropriately protective, internally consistent, cost-effective and to address the RA with greater accuracy and precision when going from lower to higher tiers.
- A reference tier is considered, based on the most sophisticated experimental or modelling method that addresses the specific protection goal, and then this reference tier is used to calibrate lower tiers using simpler methods that are practical for routine use (EFSA 2010a).

Furthermore, SPGs might be differentiated by land use, land cover or habitat type. Presumably, the protection level of natural reserves, (semi-) natural habitats, small anthropogenic habitats within cultivated landscape and in-field areas will differ. For example, plant communities of higher protection level should have a minimum spatial extent and should not be significantly affected by other factors (*e.g.*, fertiliser input, mechanical effects, mowing, etc.), as is the case for small herbaceous strips of ≈1-3 m width which frequently occur at the edge-of-the-field ('field margins').

Regulatory RA and RM in the framework of SPGs will require approaches (concepts, data and tools) to quantify the extent of effects along risk dimensions and their likelihood of occurrence.

4.3.2.2 Forthcoming and Auxiliary Regulations, Guidance and Recommendations

Besides current legislation and regulations directly referring to the authorisation and regulation of PPPs (Section 4.3.2), further European and national regulations, guidances and recommendations directly or indirectly relate to the authorisation and use of PPPs. Some of these, which relate to the goals of this thesis are briefly introduced below (without claiming completeness):

- In their discussion paper 'Addressing the New Challenges for Risk Assessment' (EC 2012b), Scientific Committees of the European Commission draw the following conclusions: "*For a number of scientific and other reasons, the procedures currently used for both human and* ecological *risk assessment are anticipated to change substantially over the next few decades. ... ECOLOGICAL RISK ASSESSMENT: The approaches in current use for ecological risk assessment are likely to suffice for regulatory purposes as sufficiently protective for ecosystems. However they lack environmental realism. … The main challenge for ecological risk assessment is to develop tools that take account of the complexity of the potentially exposed ecosystems and enable assessment of sitespecific effects.*"
- The Sustainable Use Directive (EC 2009b) aims to fill the legislative gap regarding the use-phase of PPPs (EC 2012a) through national plans for reduction of risks, including, *e.g.*, best practices in river basin management and specific protection of sensitive areas. The National Action Plan on Sustainable Use of PPPs in Germany (BMELV 2013) sets a target to reduce the risks arising from the use of PPPs by another 25% by 2020. Actions comprise Integrated Pest Management, generic RM, identification of local spots of unacceptable risk and the use of risk indicators (BMELV 2008).
- The Water Framework Directive (WFD, EC 2000) commits Member States to achieve 'good chemical and ecological status' for all groundwater and surface water bodies by 2015. The status is assessed according to biological, hydro-morphological, physical-chemical and chemical criteria. For the latter, standards are specified regarding maximum concentrations of substances (*e.g.*, of PPPs). River catchments represent RA and RM units.
- Biodiversity: "*The EU is committed to the protection of biodiversity, and to halting biodiversity loss within the EU by 2020. Over the last 25 years the EU has built up a vast network of 26.000 protected areas in all the Member States and an area of more than 750.000 km^2, which is 18% of the EU's land area. Known as Natura 2000, it is the largest network of protected areas in the world …. The legal basis for Natura 2000 comes from the Birds Directive* (DIRECTIVE 2009/147/EC) *and the Habitats Directive* (DIRECTIVE 92/43/EEC)*, ... But protected natural areas cannot thrive in isolation: if we want to conserve Europe's natural capital, then agriculture, energy and transport policies must be sustainable too."* (EC 2012c).
- The Biocidal Product Directive (Directive 98/8/EC) aims to harmonise the European market for biocidal products and their active substances. Directive 91/414/EEC on PPPs, served as a model for the new Directive (EC 2012d).
- INSPIRE Directive (EC 2007): 'Infrastructure for Spatial Information in the European Community'. The key goal is to facilitate the use of geodata across Europe by harmonisation of a range of data and system aspects, *e.g.*, requiring web-based services for visualisation and download. "*… establishing an infrastructure for spatial information in Europe to support Community environmental policies, and policies or activities which may have an impact on the environment. The Directive requires that common Implementing Rules (IR) are adopted in a number of specific areas such as: Metadata, Data Specifications, Network Services, Data and Service Sharing and Monitoring and Reporting.*" (EC 2013, GDI 2012, GDI 2013).

- The European Workshop on Probabilistic RA for the Environmental Impacts of PPPs (EUPRA, Hart 2001) aimed at, *e.g.*, reviewing the worldwide state of the art in probabilistic methods of RA, for analysing the impact on the environment of PPPs and definition priorities for further research. A list of strength, opportunities and weaknesses was set up. General agreement was obtained that probabilistic approaches provide an improved risk characterisation, yet, which can be more complex, need more data and are more difficult to communicate. "*The workshop concluded that probabilistic methods would improve the environmental evaluation of plant protection products under Directive 91/414/EEC (Remark by the author: 91/414/EEC is today replaced by EC Regulation 1107/2009, EC 2009a), provided they were implemented appropriately to minimise their potential disadvantages. This conclusion applies to all three areas considered by the workshop: aquatic organisms, terrestrial vertebrates, and terrestrial invertebrates and plants.*". The workshop reported recommendations of which a few were extracted as being closely related to the objectives of this thesis: "*Probabilistic methods should be introduced gradually to assist decision-making on the ecological risks of pesticides, beginning with those cases where they are most needed.*"; "*Probabilistic methods constitute one of several approaches that may be used for refined ("higher tier") assessments.*". The workshop identified research areas to develop probabilistic approaches, *e.g.*: extrapolation from individuals of single species (laboratory) to populations (field) and communities; variability of exposure in the landscape; regional variation in sensitivity of non-target organisms; presence of sensitive/robust life stages; quantification of the spatial distribution of different types of water bodies and their proximity to crops.
- Development of a RA of PPPs for bees (EFSA 2012a): "*For the development of robust and efficient environmental risk assessment procedures, it is crucial to know what to protect where to protect it and over what time period. … Pollination, hive products (…) and biodiversity (…) were identified as relevant ecosystem services.*" Different routes of potential exposure were identified, *e.g.*, after spray treatments in pollen and nectar, guttation droplets, dust drift; "*… the inclusion of multiple exposures with appropriate weights would need to be done with a modelling or scenario-based approach…*".
- FOCUS Working Group on Landscape and Mitigation Factors in Ecological RA (FOCUS 2007a, 2007b): A key objective of the group was to review the current state-of-the-art and to provide a general framework for refining aquatic RAs. Adoption of approaches discussed in the reports was recommended on a case-by-case basis. The group developed extensive reviews on harmonised approaches to mitigation measures, on methods and data for describing agricultural landscapes, as well as on ecological considerations in RA.
- Example regional RM at national level:
    - The Dutch regulation considers regionally adapted RM in drinking water abstraction areas (Alterra 2012) and locally adapted mitigation measures to protect water bodies (CTB 2004, in van de Zande *et al.* 2004).
    - Some of the 16 German Federal States recommend or prescribe generic buffer zones to water bodies or have implemented exemption clauses to Plant Protection Product use (*e.g.*, 'Altes Land').

- RM in Stever catchment in Germany resulted in 90% reduction of isoproturon to meet the requirements of the drinking water directive by using, *e.g.*, buffer strips, equipment cleaning points for spraying machines, and anti-drift nozzles ('*RM in a drinking water catchment area – experiences in the Stever river basin in Nordrhein Westfalen*', Frahm 2012).
- In Italy, regulations are under consideration to regionally impose generic buffer zones to water bodies depending on monitoring results (A Cantoni, Bayer CropScience, 2012, pers. comm.).

- Recommendations from workshops, working groups and conferences: In recent years, the topic of improving ecological risk characterisation, RA and RM, with particular consideration of population level and landscape-scale has been differently discussed. The development of this thesis was stimulated by the author's contributions and exchanges with experts at different occasions, *e.g.*, at SETAC EU Annual Meetings (2006-2011, SETAC 2013a), SETAC GLB (Schad 2006a), MeMoRisk (Europe Advisory Groups: Mechanistic Effect Models, SETAC 2013b), LEMTOX (Thorbeck *et al.* 2009), ModeLink (MODELINK, SETAC Europe Technical Workshop, October 2012 and April 2013), GeoPERA (Schad *et al.* 2006b, 2006c, 2007) and GeoRISK (UBA 2010).

4.3.3 General Policies and Developments

According to United Nations, the world population is projected to reach 9.3 billion by the middle of this century (UN 2011a, 2011b). This development will further increase the need for crop production, but should be done by maintaining biodiversity ("*food & biodiversity*" problem). The Food and Agriculture Organisation (FAO) promotes the concept of 'Sustainable Crop Production Intensification': "*Sustainable crop production intensification provides opportunities for optimizing crop production per unit area, taking into consideration the range of sustainability aspects including potential and/or real social, political, economic and environmental impacts. Recent trends would indicate that the incorporation of scientific principles of ecosystem management into farming practices can enhance crop production (yield). With a particular focus on environmental sustainability through an ecosystem approach, sustainable crop production intensification aims to maximize options for crop production intensification through the management of biodiversity and ecosystem services.*" (FAO 2012, FAO 2013b).

In the United Nations 'Millennium Ecosystem Assessment' (UNEP 2013) consequences of ecosystem change for human well-being and the scientific basis for action, which are needed to enhance the conservation and sustainable use of those systems, were assessed. Ecosystem Services were grouped into categories: *provisioning* (*e.g.*, production of food and water); *regulating*; *supporting* (*e.g.*, crop pollination); and *cultural* (*e.g.*, spiritual, recreational) benefits. Despite a debate on whether the concept sufficiently supports objectives of nature conservation (*e.g.*, McCauley 2006), there is general agreement that Ecosystem Services provide a powerful and effective tool in making consequences of human activities to ecosystems explicit and transparent. The approach was adapted by EFSA (2010a) as a basis for the development of Specific Protection Goals (Section 4.3.2).

4.4 Landscape-scale Aspects in Regulatory Ecological Risk Assessment and Risk Management of Plant Protection Products

"*It's the type of question that we ask at landscape scale.*" (anonymous)

In this section the meaning of the landscape-scale perspective is discussed with respect to ecological RA and RM in the regulation of PPPs (Section 4.3), as well as to scientific and methodological approaches. This perspective is linked to the discipline of landscape ecology (Wu & Hobbs 2007) from which it might be more systematically inspired in the future. The objective of this section is to build a basis upon which requirements for landscape-scale modelling in regulatory RA and RM can be formulated.

In Section 4.2, the cultural meaning of cultivated landscapes was discussed and the relationship "*Landscape = Context*" was formulated. This meaning is reflected in the range of protection, developmental and further societal goals (Section 4.3). This, together with the obvious fact that sufficient understanding and describing of (meta-) populations, communities or ecosystems *per se* requires to take an adequate abiotic and biotic context into account, including human activities. However, this does not necessarily turn the landscape-scale into an indispensable, routinely employed operational unit in risk characterisation, RA and RM of PPPs. The landscape-scale is perceived as providing sufficient and necessary context to develop tiered RA procedures with corresponding scenarios, including higher-tier options. Being in particular focus of human activities and related to administrative boundaries, the landscape-scale represents an appropriate unit for PPP-specific and generic RM measures. Selected aspects are summarised in Table 2 and are discussed in the following sections.

Table 2: Landscape-scale aspects in regulations related to ecological RA and RM of PPPs.

Topic	Landscape-scale Aspects
Ecosystem Services	Ecosystem protection goals meet at the landscape-scale which represents the integrative level. Characterisation of specific services (*e.g.*, ecological, economic) can be introduced to higher level RM decision-making.
Food production	The cultivated landscape represents the food production area. Sustainable intensification of food production. Integrated management approaches.
Water quality	Water supply quality management (*e.g.*, protection zones, catchments).
Land management	Management of landscape composition and structure (land use /cover).
Ecological Protection Goals	SPGs target at biological organisation levels (meta-) population and communities and explicitly refer to a range of spatial and temporal scales in different risk dimensions. Ecological processes are affected by a range of abiotic and biotic factors at different scales. Landscape-scale context can support the definition of risk acceptability criteria in SPGs.
Biodiversity	The overarching protection goal represents a biological organisation level that relates to a number of abiotic and biotic conditions and interactions.
Bees	Pollinators make use of a range of (dynamic) pollen, nectar and water sources across the landscape. Spatiotemporally variability of exposure to

Topic	Landscape-scale Aspects
	PPPs and further risk driving factors.
Endangered species	As with other species, risk of endangered species to be affected by PPPs depends on spatiotemporal co-occurrence of exposure and species occurrence (and activity characteristics, *e.g.*, nourishment).
Nature conservation	Management of natural reserves and their relationship to agricultural areas. Habitat quality and dynamics. Landscape Ecology.
Sustainable Use	National Action Plans to assess real-world risks due to PPP use.
Risk management	Identification and implementation of effective regional and local RM measures (generic, specific, stewardship) on the basis of local RA. Administrative units can support implementation. RM of PPPs as an integrative part of land management.
Monitoring	Human activities in cultivated landscape, as use of PPPs, and their biotic and abiotic consequences can be related and monitored at landscape-scale. Monitoring provides a basis for validation of RA procedures (models). Definition of monitoring regions and study design.
Risk assessment	Development of tiered RA schemes. PPP-specific risk characterisation and RA procedures in context to real-world biotic and abiotic processes, including human activities.
Risk communication	Visualisation and discussion of local RA in context to real-world conditions. Relationship of study and model assumptions to real-world conditions. Occurrence of Hot-Spots. Effectiveness of RM.
Scenarios	Real-world or constructed landscapes can provide the necessary biotic and abiotic context to define scenarios for ecological RA and RM.
Exposure characterisation	Mechanistic modelling of PPP use, exposure and environmental fate processes. Spatiotemporal variability and scale dependencies.
Effect characterisation	Mechanistic modelling of effects on (meta-) population and community level. Spatiotemporal distribution of species occurrence, life-stages and sensitivity. Spatiotemporal variability and scale dependencies. Higher-tier ecotoxicological studies.

4.4.1 Risk Characterisation and Risk Assessment

As the term suggests, risk characterisation is the process of quantifying risk. In ecological RA, the term *Impact* in the fundamental definition of risk, *Risk = Impact x Probability* (Section 4.3.1.1), refers to a potential extent of an adverse effect (at defined biological entity level and attribute, Section 4.3.2.1). At individual level, for an adverse effect to occur requires a sensitive species and life stage to co-occur with a significant exposure extent in space and time (r,t):

effect = f(exposure(r,t), species sensitivity(r,t)) (Equation 2)

The spatiotemporal coordinates (r,t) (where 'r' is a spatial location and 't' is time) in risk characterisation provide a first indication of the spatiotemporal variability of ecological risk due to PPP use. Ultimately, understanding this variability is a prerequisite to understanding risk under real-world conditions. This level of risk characterisation directly relates to landscape-scale as this scale covers the necessary abiotic and biotic processes and their spatiotemporal variability, *e.g.*, land use, PPP use, exposure, environmental fate, and species ecology.

However, the purpose of ecological RA in regulation of PPPs is not primary to understand risk in all its details under real-world conditions, but to assess risk acceptability with reasonable certainty. Thus, risk acceptability criteria and scenarios in ecological RA define the necessary risk characterisation level. Both are provided in tiered RA schemes (*e.g.*, FOCUS 2001, EC 2002a, EC 2002b, EFSA 2010a, EFSA 2012b) ranging from conservative lower-tiers, with clear and detailed definitions and instructions, up to higher-tiers of less prescriptive and a more recommendatory framework. Lower-tier RA schemes are simple and are conservatively designed to represent a 'realistic worst case', aiming at the identification of PPP uses of low risk ('true-negatives'). Thus, lower-tier levels are *per se* not defined for quantitative risk characterisation under more realistic conditions. In case a lower-tier RA level indicates unacceptable risk, refined risk characterisation and RA is necessary.

4.4.1.1 Recent Developments in Landscape-scale Risk Characterisation and Risk Assessment

The general need for an improved quantification of risk has been recognized on various occasions, *e.g.*, in working groups of FOCUS Landscape and Mitigation (FOCUS 2007a, 2007b), the EUFRAM project (Hart 2006), projects of the German Federal Environment Agency (UBA, GeoRISK, UBA 2010; Schulz *et al.* 2007, 2009), a project of the German Crop Protection Association (IVA, GeoPERA, Schad *et al.* 2006b, 2006c, 2007), work of the Julius Kühn Institute (JKI, Golla *et al.* 2008a, 2008b, Strassemeyer *et al.* 2009), as well as in specific RA (Maund *et al.* 2001, Hendley *et al.* 2001, Travis and Hendley 2001, Wang and Rautmann 2008). With respect to the introduction of probabilistic approaches, the focus of recent projects was mainly on 'the effect side' of the risk equation, *i.e.*, addressing variability and uncertainty in the toxicity of a substance, *e.g.*, due to experimental design or intra- and interspecies variability (EUFRAM, Hart 2006). Because the variability of risk is largely driven by spatial and temporal variability of environmental and agricultural conditions that affect the spatiotemporal distribution of exposure and susceptible populations (Verdonck 2003), the use of geoinformation has become a prominent tool in recently refined RA approaches (Travis and Hendley 2001, Padovani *et al.* 2004, Schad *et al.* 2006b, 2006c, 2007, Golla *et al.* 2008b, Schulz *et al.* 2007, 2009, Strassemeyer *et al.* 2009). With the work of the FOCUS Landscape and Mitigation group (FOCUS 2007a, 2007b), basic aspects of landscape-scale study designs have been evaluated and recommendations have been made. In recent years, different spatially explicit studies aiming to refine exposure assessment have been conducted using geodata to refine factors such as the crop-to-WB distance or the possibility of different wind directions. Early studies were more focused on the quantification of the crop-to-WB co-occurrence in order to put the occurrence of standard scenario assumptions into the context of real-world conditions. In more recent approaches, calculations on local spray-drift deposition were done in order to derive a 'landscape-scale' realistic worst-case PECs (Padovani *et al.* 2004, Schad *et al.* 2007, Schulz *et al.* 2007, 2009); however, in only a few studies steps have been taken toward probabilistic analysis in a narrower sense (Wang and Rautmann 2008, Golla *et al.* 2008b, Golla *et al.* 2011). In the past decade, progress in spatially explicit studies has mainly been due to the increased availability and affordability of data (such as high-resolution satellite imagery and topographic data), the technology for processing geodata (Geographic Information System (GIS) tools), and increased computing power. Large models (Morgan & Herrion 2007) have emerged which aim at covering a large range of landscape factors in order to assess the impact of land use dynamics and land management (including PPPs) on animal species (*e.g.*, population dynamics) using real-world geodata and a number of processes (*e.g.*, Pastorok *et al.* 2002, Wu & Hobbs 2007, Topping 2009).

Furthermore, the process of refined ecological risk characterisation is currently stimulated by a number of research fields, in particular improved mechanistic effect modelling (ModeLink (SETAC Europe Technical Workshop, October 2012 and April 2013), ELink (Brock *et al.* 2009), EC 2012b) and higher-tier effect assessment (*e.g.*, Wolf *et al.* 2010).

4.4.1.2 Future Developments in Landscape-scale Risk Characterisation and Risk Assessment

As indicated in Section 4.3.2 and 4.3.3 and summarised in Table 2, current and future developments in regulations and regulatory science related to PPPs suggest a next generation of landscape-scale concepts and approaches in risk characterisation. The following aspects were identified as important in the next development steps of ecological RA and RM:

- Consistent concepts and approaches for RA problems of structural similarity.

  This suggests a sufficiently generic approach, which is adaptable to similar RA problems in SPGs context, concerning, *e.g.*, environmental compartments, exposure routes, effect endpoints of risk dimensions (Section 4.3.2.1) and context levels (below).

- Explicit consideration of context levels (*AutContext*, *SynContext*, Figure 3, Section 4.2) in relationship to PPP-specific RA and generic RM, including transition levels.

- Potential for stepwise introduction of context and complexity in risk characterisation ('*from protective to predictive*') including abiotic and biotic conditions, as well as human activities (land use, land management).

  This, stepwise approach should be considered in higher-tier approaches as well as in scenario development of quantified protection levels for future tiered RA schemes. Stepwise approaches towards higher complexity levels are necessary to ensure association and consistency with current RA and RM schemes and traceability of risk characterisations.

- Consideration of the fundamental definition of *risk* (Section 4.3.1) in risk characterisation.

  This includes probabilistic approaches. The propagation of variability (and uncertainty) by the model should comply with the fundamental paradigm of probabilistic approaches (Section 4.5.5).

- Explicit consideration of scales in space and time in all assessment steps (*e.g.*, landscape factors, model input parameter variability, model outcome and ecological risk characterisation, RA and RM, '*risk has scales*').

- Application of the landscape-scale perspective as unit of analysis (real-world conditions, scales, structure, ecology) and as integrative unit of assessment in the Ecosystem Services framework.

- Application of appropriate technological means to manage the inherent complexity of landscape-scale approaches.

4.4.2 Landscape-scale Context in Plant Protection Product-specific Risk Assessment

Authorisation of PPPs in European Member States is based on *Indication*, which specifies the use of a PPP in certain crops against certain pests including application guidelines (*e.g.*, BMELV 2012). The *Indication* is legally binding and is printed on the product label.

Correspondingly, regulatory RA for a certain PPP is basically *Indication*-based. For example, for a PPP that is intended to be used in apple cultivations with specified applications (number, use rate(s), application interval, etc.), RA for this PPP essentially focuses on the specified use.

Current standard (lower-tier) RA scenarios and their risk acceptability criteria are adapted to this principle by basically following (realistic) worst-case principles in order to establish protective scenarios, *e.g.*, referring to the edge-of-the-field-scale (FOCUS 2001, EC 2002a, 2002b, EFSA 2012b). As such, the scenarios focus on the identification of 'true negatives', *i.e.*, PPP use of low risk, but are not intended for quantitative risk characterisation. The latter, however, will be required in particular with respect to future SPGs (Section 4.3.2.1) which require more context in scenario definitions (Reference Scenarios, EFSA 2010a).

Therefore, the problem arises of how to set an *Indication*-based risk characterisation, RA and RM in a larger landscape-scale context, ultimately taking the range of relevant processes into account which affect Non-Target-Organisms ('*Indication-Context Problem*', Section 4.2, Figure 3). A straightforward solution barely exists, as there are inherent limitations, *e.g.*, a notifier conducting a risk characterisation does not have the context regarding other PPP uses. This, and further regulatory constraints were identified in the GeoRISK project of the German Federal Environment Agency (UBA 2010) in which regulation of *Indications* were set in context to *generic* RM measures at regional and local scale, or earlier by the work of the FOCUS Landscape & Mitigation Group (FOCUS 2007a, 2007b).

Therefore, and as risk characterisation, RA and RM in larger landscape-scale context is in its infancy, at present, heuristic case-by-case approaches are proposed taking available experiences in RA into account. The following preliminary proposals are intended to support a stepwise introduction of landscape-scale context to PPP-specific RA problem formulations:

- Starting at lower-tiers: Results of lower-tier RA steps and their scenario definitions could serve as starting point for a stepwise implementation of improved environmental and ecological context.
- Simplicity: Studying simplicity improves its transparency. This can be achieved, *e.g.*, by keeping the definitions of lower-tier and only refining landscape factors driving risk (exposure, effects, variability).
- Conservatism: Maintenance of an overall conservatism of study definitions; hence, results assure an inherent protection level which can cover remaining uncertainties.
    - Use conservative scenario definitions from lower-tier(s) in exposure calculations (*e.g.*, WB definitions, spray-drift deposition in terrestrial habitats). This also applies to refinements from landscape analysis, *e.g.*, taking a generic crop type ('orchards', 'arable') as the occurrence of the actual specific type of the *Indication*.
    - PPP use: *e.g.*, 100% use of the target PPP (100% market share) at 100% of the target crop (all crop treated).
    - Conservative aspects in effect assessment, *e.g.*, lower-tier ecotoxicological test design, assessment factors, and parameter settings in population modelling. In absence of data on species occurrence, general occurrence of the sensitive species and life stage(s) in space and time can be assumed.
    - Study region spatial extent focused to cultivated area of a region plus direct (natural) surrounding of direct ecological relationship to the cultivation area in order to avoid 'artificial effect dilution'.
- Scope: Landscape-scale context often refers to specific real-world study regions. The characteristics of these regions, and the findings based upon these with respect to their representativeness and conservativeness for the entirety of cultivation conditions in a Member State or in Europe can be quantified using indicators (landscape metrics, McGarigal & Marks 1995, *e.g.*, Section 6.1).
- Background context: Explicit landscape factors affecting Non-Target-Organisms can be 'phenomenologically' introduced, *i.e.*, not by explicit mechanistic modelling but as implicit 'background' phenomena.
    - Spatial extension of the targeted *Indication* to further uses of the target PPP. For example, the *Indication* refers to apple, but if the PPP is also used in cereals, then both crops can be considered.
    - Temporal extension of the targeted *Indication* as part of a sequence of PPP measures. Other PPP uses in the target crop are replaced ('*inter pares*') by the *Indication*.
    - Population background mortality or sublethal effects (phenomenological).
- Supportive use: Outcome of landscape-scale risk characterisation can support the overall RA on the basis of all available evidence.

Some of the preliminary proposed approaches are considered in the case studies (Section 6) which demonstrate the added value of landscape-scale risk characterisation under the constraints given by the *Indication-Context Problem*. A developing empirical basis of landscape-scale risk characterisations can support the development of long-term solutions to the problem. The fundamental meaning of the '*Indication-Context Problem*' suggests further research is needed in scientific (*e.g.*, exposure and effect modelling, habitat quality, abiotic and biotic geodata) and regulatory disciplines. Computing resources are not a principle constraint to detailed context in landscape-scale risk characterisations ('Cloud Computing', *e.g.*, Windows Azure, Microsoft 2013).

4.4.3 Risk Management

Landscape-scale approaches are of immediate use to assess the effectiveness of alternative RM measures and their cost due to spatially (and temporally) explicit risk characterisation on the basis of more realistic (real-world) conditions. This applies to basically all aspects of RM:

- <u>PPP-specific mitigation measures</u>: *e.g.,* adaptation of PPP use rates and frequencies, application timing, use of drift reducing technology, buffer zones, etc.
- <u>Generic regional RM</u>: *e.g.,* WB maintenance, windbreaks, vegetated buffer strips, constructed wetlands, habitat quality, land management, conservation areas.
- <u>RM at different scales</u>: Local habitat segments of high potential risk ('hot-spots') can be identified and management options investigated. Application technology using Global Positioning Systems (GPS) can adapt PPP use to local habitat vulnerability (precision farming, *e.g.*, ISPA 2013). Regional measures can manage, *e.g.*, water quality in a catchment or biodiversity of plant or arthropod communities.
- <u>Integration of RM measures</u>: The landscape-scale allows to integrate societal goals from different Ecosystem Services perspectives (*e.g.*, ecological and economic risk) and so to implement concerted actions (*e.g.*, Water Framework Directive, Sustainable Use Directive, Section 4.3.3).
- <u>Monitoring:</u> Landscape-scale risk characterisation can support the identification of monitoring sites and the definition of spatiotemporal sampling density, as well as the explanation of monitoring findings (*e.g.*, identification of most likely exposure sources).
- <u>Cost:</u> Effective RM is a prerequisite to achieve ecological protection goals at sensible cost.
- <u>Risk communication:</u> Explicit landscape-scale risk characterisation and can serve as a means for risk communication to decision makers and public (*e.g.*, translating complex concepts and results using maps). The immediate relationship to the real-world entities provides a transparent basis for expert or public examination.

4.4.4 Outlook on Explicitness in Risk Assessment and Risk Management

If not excessively unrealistic, an imaginary outlook can help to reflect possible consequences of developments, and so, to steer development into agreed paths.

A superior quality of landscape-scale risk characterisation is that it makes risk more *explicit*. This has two major consequences:

i. Landscape-scale risk characterisation leads to a better understanding of risk.
ii. Improved predictive power of risk characterisation requires acting on risk.

The first consequence is generally perceived as positive and can be regarded as a natural and expected consequence of scientific development. The second, however, carries two facets:

a. Refined and more effective RM options.
b. Statements on explicit risk acceptance (*i.e.*, ecological effects + probability to occur).

On the assumption of a 'zero risk attitude', difficulties in risk acceptability by risk managers and with risk communication to the public can occur which are already being discussed in the context of the introduction of probabilistic approaches (*e.g.*, at EUFRAM project, Hart 2006). Here, with respect to landscape-scale probabilistic approaches, these difficulties are even larger as risk characterisation is georeferenced.

Despite practical difficulties, point (ii) (a, b) irreversibly points in the direction of potential future developments: when putting today's existing or realistically envisaged puzzle pieces together (*e.g.*, landscape-scale exposure, eFate and ecological modelling, geodata availability or production possibilities, Cloud Computing, service endpoints, mobile internet, cognitive systems, Google), a mosaic on future risk characterisation capabilities of <u>steadily increasing predictive power</u> occurs.

Thinking further out, as a thought experiment, an <u>ideally predictive tool</u> can be imagined, capable of predicting ecological risk due to PPP use in necessary context and at relevant scales (compared, *e.g.*, to weather forecast, or traffic jam prediction 'Watson', IBM 2012). Indications on developments in this direction can be found in Information Technologies but also in requirements from authorities, *e.g.*, in a statement of the European Commission on 'Shared Environmental Information System' (EC 2012e): "…*This is why it is absolutely vital for the European Union to have an information system based on the latest information and communication technology (ICT) that will provide decision-makers at all levels (local to European) with real-time environmental data, thus allowing them to make immediate and life-saving decisions.*"

Preliminary aspects and implications of this imaginary predictive tool are:

- Distinct <u>real-word risk acceptance</u> at known locations and times, with new requirements for risk communication. If not explicitly under data protection, which is *per se* not the case for environmental information (*e.g.*, INSPIRE, Freedom of Information Act (FOIA, USDOJ 2012)), information and knowledge derived will be public (*e.g.*, 'Information society', Wikipedia.org).
- Increased <u>transparency</u> in RA and RM decision-making ('*demystification of RA*').

- Distinct regional RM measures with new options for Integrated Pest Management in relation to developments in the field of Sustainable Intensification (FAO, Section 4.3.3), yet, also with potential consequences to regional crop production conditions and cost.
- Different regulatory context for RA of specific PPPs (*Indications*, Section 4.4.2) due to assessment in context to, *e.g.*, broad ecosystem processes or other plant protection measures in a region (*SynContext*, Section 4.2). The number of disciplines and parties affected and the complex nature of this situation has been discussed in a large project in Germany, on linking generic and PPP-specific RM for aquatic systems (GeoRISK, UBA 2010, GeoRISK-Workshop (2009) at UBA, Dessau, GeoPERA, Schad *et al.* 2007).
- Iterative definition of risk acceptability criteria and extent based on experience ('*a posteriori*'). As predictive power increases, estimates on environmental and ecological consequences become more realistic which increases the knowledge base to reconsider real-world risk acceptability, and hence, RA criteria (*e.g.,* scenario, trigger).
- A predictive tool on ecological risk can become a component (a service) of a broader Ecosystem Services assessment system in order to raise the RM level into broader socioeconomic context.
- With the associated development of contributing disciplines and their separation into services, the role of the experienced 'holistic ecological risk assessor', as acting in current RA and RM schemes, might change. In a complex system of multiple disciplines, services and layers, a single person will hardly master the entirety of involved processes, tools, data and their interaction.
- An explicitly predictive tool can basically provide any detail on risk. 'Complexity filters' by expert judgement or lower-tier approaches can decrease; hence, complexity can increase at higher decision levels, which brings new challenges to decision makers.

4.5 General Requirements to a Landscape-scale Model for Risk Characterisation

In the preceding section (Section 4.4), the role of landscape-scale approaches in regulatory ecological RA and RM of PPPs was explored. A landscape-scale model which is designed for such regulatory purposes needs to fulfil some general requirements. These are presented in this section. The general requirements were used to define specifications for the model which was developed in the course of this thesis (Part 2, Section 5).

In Table 3, major general requirements for a landscape-scale model for risk characterisation in regulatory RA and RM of PPPs are summarised (more details in following sections).

Table 3: Major general requirements for a landscape-scale model.

Topic	General Requirement
Regulatory context	Clear focus in model concepts and architecture towards use in regulatory RA and RM. Consideration of agreed procedures, *e.g.,* tiered approach, conservatism, consistency. Capability to use agreed process models. Comprehensible risk communication. Consideration of model verification and validation in context of the model purpose. Core functionality should reflect the main problem structures in ecological risk characterisation, RA and RM, with particular relationship to SPGs. Adaptability of core functionality to specific RA problems.
Landscape context	Capability to process landscape factors (geodata) relevant to risk characterisation at multiples scales and defined complexity levels, *i.e.,* option to stepwise increase the number of factors and processes.
Risk characterisation	Explicit quantification of risk ('*Impact x Probability*', Section 4.3.1.1) taking different risk dimensions into account (SPGs, Section 4.3.2.1). Spatiotemporally explicit, probabilistic approach to propagate variability of landscape factors to variability of risk, considering scale dependencies. Outcome to fit to ecological RA and RM problem.
Scales	Explicit consideration of multiple scales in entire risk characterisation (*e.g.,* variability of landscape factors, propagation of variability and uncertainty, aggregation of outcome, RA, RM).
Adaptability, Complexity, Development	Model adaptability regarding conceptual (above) as well as technical aspects which include flexibility in process description and input data, as well as scalability. The inherent complexity of landscape-scale modelling has to be managed by using modular approaches. Potential future developments with respect to increased predictive power and in context of Ecosystem Services have to be considered.

4.5.1 Regulatory Environment

The regulatory environment of a landscape-scale model is described in Section 4.3. Regulatory RA and RM of PPPs define approaches for effect and exposure assessment as well as general assessment schemes (*e.g.,* EC 2002a, 2002b, EC 2009a, EFSA 2012b, FOCUS 2001, FOCUS 2007a, 2007b, Rautmann *et al.* 2001). Generally agreed schemes include, *e.g.,* tiered approaches, scenario conservatism, consistency, transparency, harmonisation, etc. Besides available regulations and guidance, current developments in regulatory research (*e.g.,* ELINK (Brock *et al.* 2009), EFSA 2010b, EC 2012b, ModeLink (SETAC Europe Technical Workshop, October 2012 and April 2013)) provide recommendations and indicate future requirements. The range of factors affecting model development in regulatory context, and hence, the model scope, is illustrated in Figure 5.

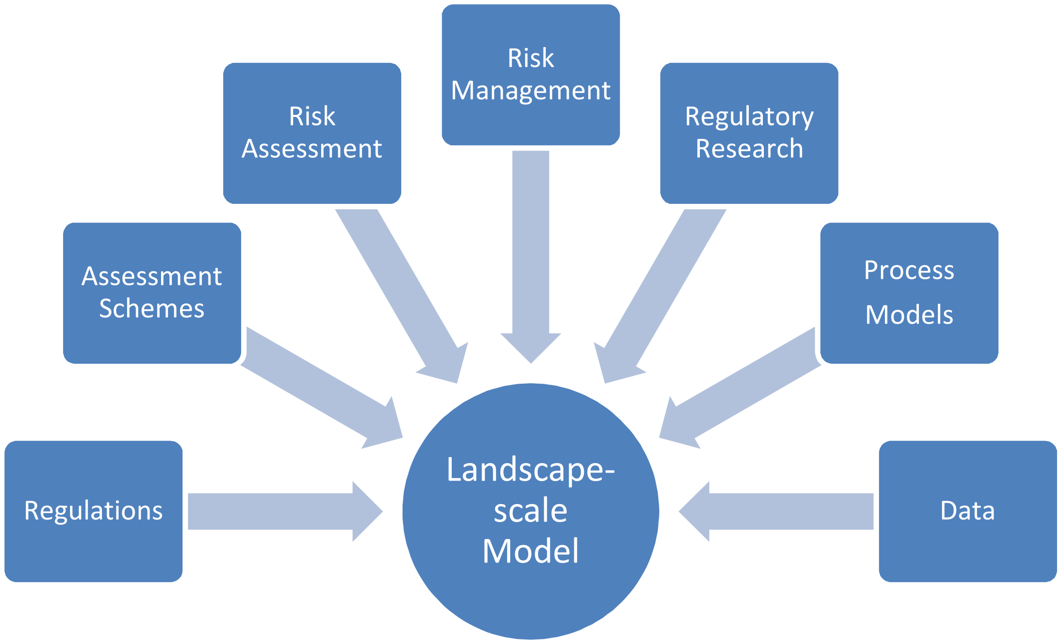


Figure 5: 'Environment' of a landscape-scale model used in regulatory framework.

Thus, a landscape-scale model approach, its concepts, architecture and implementation, for refined risk characterisation has to consider basic regulatory requirements and available process descriptions (*e.g.,* exposure, eFate, effect models). In this framework, the focus of a landscape-scale model is less in developing new process description, but in the introduction of more context (data, scales, variability) to risk characterisation. Thus, the model can be regarded as a <u>landscape-scale context-setting effort of existing model approaches</u>. Particular attention has to be paid to a comprehensible communication of refined risk characterisation based on model outcome.

With their harmonised conceptual design and categorical risk dimensions, SPGs (EFSA 2010a, Section 4.3.2.1) indicate that ecological RAs of PPPs share a basic problem structure (*e.g.,* Risk Dimensions, scales, exposure and effect assessment, risk definition). Thus, the core approaches of the model should reflect the main problem structures in ecological risk characterisation, RA and RM, while being adaptable to specific RA problem formulations.

Ecosystems have an inherent complexity (Levin 1998). In a regulatory decision-making process this natural complexity need to be reduced and managed. This applies to the development process of SPGs from general policies (Section 4.3.2) as well as to each individual RA process step. Landscape-scales models are *per se* exposed to real-world complexity levels, as they operate with real-word data and typically take a number of processes into account. Therefore, the need to reduce real-world complexity in the regulatory framework is reflected in the landscape-scale model. The landscape-scale model as a risk characterisation unit can be regarded to take an intermediary role between the complex real-world and the simple RM decision structure (Figure 6). Thus, the model architecture and design need to reflect the structure of landscape-scale inputs (data, processes) and need to structure its outcome according to risk characterisation, RA and RM requirements. The latter comprises, *e.g.*, an adequate aggregation of model outcome according to ecological protection goals, RA schemes and RM practices, taking rules of risk communication into account (Section 4.3.1.4).

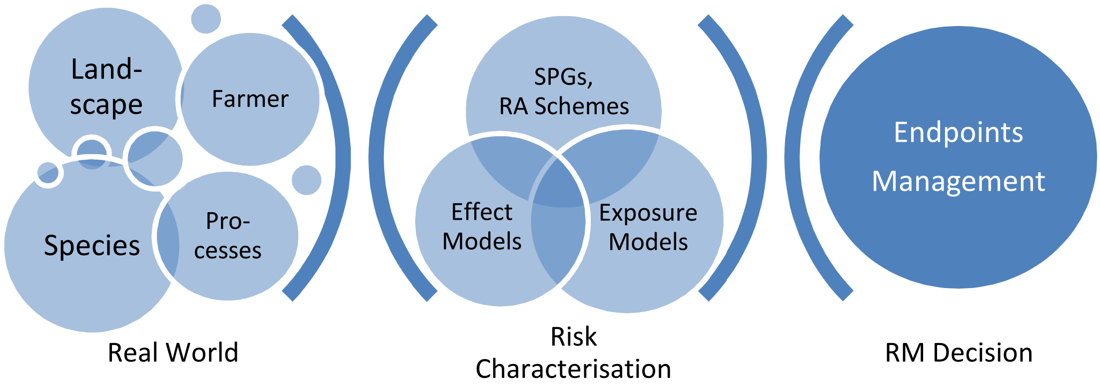


Figure 6: Schematic complexity reduction in the RA and RM process with the landscape-scale model as a risk characterisation unit between the complex real-world and the simple RM decision structure.

A model is designed for a certain purpose. Depending on the role of a model in a decision-making process (*e.g.*, informative, supportive, decisive) consequences are derived or are at least influenced by the model outcome. This model environment also indicates a corresponding definition of model validation. Model verification should test the system against the range of functional and non-functional requirements including technical aspects. Model validation refers to the usefulness of the model with respect to the intended purpose, here, in addressing a given RA problem within a given RA tier. Basically, even without explicit use of mathematical models, regulatory RA schemes make use of (more implicit) model representations as simplifications of the real world. Replacing or extending these by explicit use of mathematical models doesn't change the fundamental regulatory RA schemes and objectives, but indicates the use of a model for a certain purposes. In this perspective, validation should consider, *e.g.,* model verification (above) and a scientific review of model concepts, approaches, and scenario assumptions, as well as assessing the model 'behaviour' against expert knowledge.

4.5.2 Landscape Context

The general objective of a landscape-scale model is to improve the quantification of risk by increasing the real-world (landscape) context. In regulatory RA, risk characterisation should not include other factors than such driving risk, in order to keep the complexity within limits. Landscape context can comprise, *e.g.,* land use and land management, habitats of Non-Target-Organisms, cultivation practice (including PPP use), landscape structure, abiotic environmental conditions affecting exposure, eFate and effects, or more complex biotic interactions.

The model should allow to introduce such real-world context at different complexity levels (levels of realism) depending on the goals of an assessment, *e.g.,* a PPP-specific RA problem formulation or a generic scenario development effort for a defined RA tier. Even within a single RA problem, a stepwise increase of realism (complexity) can be appropriate, *e.g.,* in order to keep the approach consistent with current lower-tier RA schemes and to assure traceability of outcome.

Besides providing input data for model process parameterisation, the landscape-scale represents the context into which the model can map its outcome ('*landscape context → model → landscape context*'). This is of particular importance to RM and can be regarded as part of the risk communication. Thus, on the one hand, a landscape-scale model needs to reflect the general structure of ecological RA and RM problems (Section 4.5.1). On the other hand, the model need to be sufficiently flexible to be adapted to specific representation of landscape context at different complexity levels as resulting from specific RA and RM problem formulation.

4.5.2.1 Geodata

The explicit use of geodata is among the primary characteristics of a landscape-scale model approach. The geodata used in a risk characterisation are an important determinant of the scope of a study. Different geodata can be sensibly employed in landscape-scale risk characterisation (examples in Section 6). Geodata applicability depends on problem formulation (*e.g.*, thematic and spatial resolution, scale, etc.). In ecological RA, necessary geodata include *e.g.*, land use, land cover, species habitats, weather, agricultural practice, hydrology, elevation, soil, species occurrence (*e.g.*, Biggs *et al.* 2005), etc.

Acquisition and preparation of geodata can be a cost intensive part of a landscape-scale risk characterisation. In recent years, the availability of geodata and its accessibility have significantly increased across Europe, partly as a result of European policies (*e.g.*, INSPIRE Directive, EC 2007). Conventional land use / cover and topographic data (*e.g.*, ATKIS, BKG 2006, CTR 2006, CTRN 2012) as well as weather and soil data can be accessed from institutions and are regarded as 'base geodata'. A major step forward was made with the emergence of high-resolution remote sensing imagery (*e.g.*, Satellite Imaging Corporation 2012, Astrium 2012, GeoContent 2012, BKG 2012, Microsoft BingMaps shipped with ArcGIS, ArcGIS Online (ESRI 2012), Google 2012, etc.) and the development of object-based image analysis software (*e.g.*, Trimble 2012, Exelis 2012). Application of remote sensing data emphasises the necessity to consider scale effects in the risk characterisation process (*e.g.*, Quattrochi & Goodchild 1997).

Often, 'base geodata' can be introduced to the assessment by making additional (conservative) model assumptions: *e.g.*, the conservative assumption can be made that a sensitive mite species occurs in all LULC types representing semi-natural habitats (although the actual distribution of occurrence of the species is limited to habitats of certain quality only). Furthermore, if the necessary data do not exist and cannot be generated at reasonable cost, study goals and scope might be adapted to fit to the data potential (*e.g.*, regarding thematic resolution or scales). In case the RA problem formulation is of broader interest, and as geodata is *per se* generic (*i.e.*, is not related to a specific PPP), joint efforts for harmonised geodata development can be a result of a preliminary refined risk characterisation at landscape-scale. Thus, landscape-scale risk characterisation and geodata development can interact to their mutual benefit (*e.g.*, IVA GeoPERA project, Schad *et al.* 2006b, 2006c, 2007).

In the context of a landscape-scale risk characterisation, processing of geodata in a Geographic Information System (GIS, *e.g.*, ArcGIS, ESRI 2012) generates required model input data (*e.g.*, target fields for PPP application, aquatic habitats and vegetated buffer strips in-between).

The core logic of a landscape-scale model for risk characterisation should be independent from the geodata used and their preparation process. The geodata source should be regarded as a service, behind which geodata preparation steps are masked.

Besides selection of appropriate geodata attention has to be paid on the definition of the spatial scope of a risk characterisation. The definition of study region(s) depend on the RA problem formulation (case studies, Section 6). The model should be scalable to operate with different spatial data extents.

4.5.2.2 Agricultural Practice

Agricultural practice can be considered to (dynamically) affect habitat quality of species, hence, species population dynamics (Section 4.2). This is mimicked in complex landscape simulation systems like ALMaSS (DCE 2012, "*The Animal, Landscape and Man Simulation System is a landscape scale simulation system for investigating the effect of changes in landscape structure and management on the population size and distribution of animals in the Danish landscape*"). Depending on the ecological RA problem formulation, agricultural practice and land management can represent driving factors in risk characterisation of PPPs (*SynContext*, Figure 3, Section 4.2).

A landscape-scale model for refined risk characterisation of PPPs in regulatory RA and RM framework should allow to model agricultural practice at different complexity levels. This is proposed to be done stepwise, *e.g.,* starting with the PPP use in focus (Indication, Section 4.4.2) and extending the plant protection measures to multiple PPPs used in multiple crops at multiple times. Simple agricultural practice can also include crop rotation. The model should be flexible to cover further refinements, *e.g.,* concerning field management like sowing, tillage, harvesting, or alternative plant protection measures. Land management practice can also comprise maintenance of ditches or riparian vegetation. The latter has proven important as a filter for spray-drift depositions into water bodies (Section 5.3.5.5).

Variability of agricultural practice needs to be represented at appropriate spatiotemporal scales (*e.g.,* time windows for PPP uses, cropping). The 'field', the 'farm' and the 'region' are among the proposed units to describe agricultural activities, hence, to define their variability.

4.5.3 Scales

Scale dependence of risk is an important topic in ecological risk characterisation, RA and RM (EFSA 2010a). The model should be capable to explicitly operate at a range of spatial and temporal scales (typically of hierarchical nature) and to aggregate its outcome to ecologically relevant scales. The definition of relevant spatiotemporal scales depends on the RA problem. Scale dependence is of particular interest to the characterisation of variability (definition of PDFs) and its propagation in model processes (*e.g.,* sampling of PDFs in a Monte Carlo approach). Biological organisation levels, as addressed in SPGs (EFSA 2010a, Section 4.3.2.1), provide further scales to be considered in refined risk characterisation.

Example spatiotemporal scales of characteristic entities and processes present in ecological RA are illustrated in Figure 7.

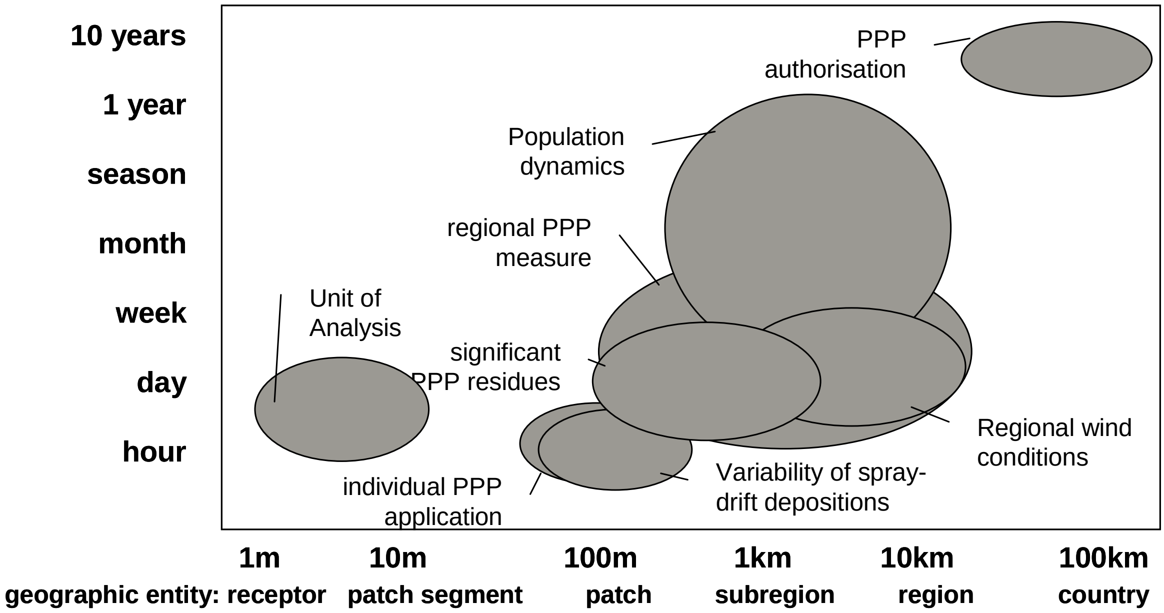


Figure 7: Schematic illustration of spatiotemporal scales of example entities and processes in ecological RA ('receptor' = smallest unit of analysis, 'patch' = individual habitat or field).

4.5.4 Variability and Uncertainty

Variability of risk of Non-Target-Organisms due to PPPs is largely driven by spatial and temporal variability of environmental and agricultural conditions that affect the spatiotemporal distribution of exposure and (sensitive) species (*e.g.*, Verdonck 2003, Section 4.4). Thus, propagation of variability of risk driving factors to risk characterisation is a key requirement to the model. This is proposed to be achieved by using two means:

i. <u>Resolving variability</u>: Explicitly resolving variability by numerical discretisation of continuous landscape factors (model input parameters) in space and time at a local scale at which variability is significantly reduced (smallest units of analysis in [time, space], *e.g.*, [day, 3x3m^2]). For example, regional variability of local crop-to-water body distance disappears when conducting model calculation at the scale of the smallest unit of analysis. Same applies when *e.g.,* assuming a fix wind direction at the time of a PPP application at a single field (space). Thus, spatiotemporally explicit landscape-scale modelling can significantly reduce remaining variability in the calculations, and hence, reduce potential correlations between landscape factors. The spatiotemporally explicit model results are subsequently aggregated at ecologically meaningful spatiotemporal scales according to problem formulation and SPGs.

ii. <u>Representing variability in PDFs</u>: Variability can be represented in PDFs (or PMFs). For example, variability of spray-drift depositions close to a treated field can be represented in a PDF, which is sampled at the local scale of the smallest unit of analysis. Sampling can be done using a Monte Carlo approach. Scale-dependencies of variability represented by PDFs (or PMFs) have to be considered.

A prerequisite to any approach resolving variability is to previously define a smallest unit of analysis ('receptor') in space and time according to problem formulation (*e.g.*, [day, 3x3m^2]) and spatiotemporally explicit model design.

The model purpose in a regulatory RA environment guides its design (Section 4.5.1); tiered RA schemes determine the simplifications of reality. Thus, effects of model uncertainties are primary to be evaluated on the background of its purpose. This needs to consider the circumstance that models are the main tools to provide the requested risk characterisations to RA questions. The model should be capable to propagate parameter uncertainty (which often include expert judgement) to model outcome, *e.g.*, by using a 2-d Monte Carlo approach (*e.g.*, Morgan & Henrion 2007, Warren-Hicks & Hart 2010). Scale-dependent and hierarchical evaluation of impacts of parameter uncertainty to model outcome has to be considered.

4.5.5 Probability

As introduced in Section 4.3.1.1 and 4.4, risk depends on stochastic events which govern the co-occurrence in space and time of significant concentrations of an active substance and a species sensitive life stage. Risk characterisation using a landscape-scale model therefore, need to account for probabilities of predefined *Impacts* to happen.

Two major interpretations of *Probability* are commonly distinguished (Section 4.3.1.1): (i) the frequentist view (empirical), and (ii) the subjectivist view (Bayesian view). The frequentist approach using Monte Carlo is proposed for numerical risk characterisation using a landscape-scale model. The outcome of the model, *i.e.,* the improved quantification of risk, can be regarded as a component to improve the state of knowledge in RA and RM (subjectivist or Bayesian view).

By taking scale-dependencies in the representation of variability into account (Section 4.5.2) the model should enable risk characterisations which comply with the central paradigm of probabilistic approaches, stating that each combination of parameters used as input vector of a trial (simulation run) should represent a case that can occur in the real-world (Vose 1996). A visual explanation to this requirement is given by Cressi & Wikle (2011): "*You are here. what happens north, south, east, or west of you is very likely to be (positively) dependent on what is happening here. This expresses a "law of Geography" that says nearby things tend to be more alike than those far apart. "Why? Because there is a flux of causal relationships in the space-time continuum that, when integrated out over time or captured in a mirco-instant of time, shows neighboring values to be more highly correlated."*. "*…spatio-temporal data should not be modeled as being statistically independent. … an assumption that spatio-temporal data follows the "independent and identically distributed" (iid) statistical paradigm should typically be avoided*".

4.5.6 Technical Aspects

The model needs to provide a core functionality aiming at a refined quantification of risk and framed by the general structure of ecological RA of PPPs (previous subsections above). At the same time, the model needs to be adaptable to specific RA problems, ecological target groups and their habitats (*e.g.*, NTA, NTTP, aquatic invertebrates, bees), data, processes descriptions (*e.g.*, cultivation practices, exposure, eFate, effect), scales and Assessment Endpoints.

The spatial extent of landscape-scale risk characterisation can range from local edge-of-the-field, to regional, and up to country-wide assessments. Thus, the model should be scalable in order to operate with small and large datasets.

The landscape-scale model can be regarded to take an intermediate role between the complex real-world and the simple structure of RM decision-making (Section 4.5.1, Figure 6). Thus, the model has to manage a considerable complexity including the capability to aggregate its outcome in order to provide a comprehensible risk characterisation for RA and RM. In this respect, the following technical means should be considered in the model development:

- Explicit representation of real-world entities (*e.g.*, farming, habitats, environmental compartments) and processes (*e.g.*, PPP use, exposure, eFate, effect).
- Explicit representation of risk dimensions (Section 4.3.2.1) and scales.
- Data aggregation steps within risk dimensions at different scales.
- Modular architecture taking service-orientation into account. Besides directly affecting the management of complexity, modularity can also support an increase of the model complexity towards increased predictive power ('*from protective to predictive*', Section 4.4.1.2).
- Simplicity as a guiding implementation principle.
- Clear representation of model entities in the model configuration.

5 Part 2: Xplicit – A Modelling Framework for Landscape-scale Risk Characterisation

This section presents a modelling framework for landscape-scale risk characterisation and its development process. The modelling framework was intended to implement the general requirements formulated in Part 1 (Section 4). The section begins with a presentation of the software development methods employed in the Xplicit development project. The two following sections present the *Xplicit-Framework* and specific ready-to-use *Xplicit-Models* derived from the framework.

5.1 Introduction

Mathematical modelling has become a prominent tool in research, applied science, engineering and regulatory decision-making (Wikipedia.org). Physicists test their theories, sociologists investigate social phenomenons, meteorologists predict weather and climate change, ecologists study dynamics in biodiversity, 'system biologists' investigate cell behaviour, and engineers simulate product properties. Even in products used in everyday life mathematical models work in the background, *e.g.*, in navigation or car safety systems.

Mathematical models play a key role in understanding and managing ecosystems in general and in ecological RA in particular (*e.g.*, Jørgensen *et al.* 1996, Pastorok *et al.* 2002, Suter 2007, Thorbeck *et al.* 2009). With an early focus on exposure modelling, mathematical models have become a prominent role in regulatory environmental and ecological RA and RM of PPPs (Section 4.3.2, *e.g.*, FOCUS 2001). Currently, mechanistic ecological modelling is evaluated for its use in regulatory ecological RA and RM (*e.g.*, Thorbeck *et al.* 2009, ModeLink, SETAC Europe Technical Workshop, October 2012 and April 2013).

Objectives and purposes of landscape-scale modelling in the regulatory decision-making process of PPPs were discussed in Section 4.4 and 4.5. The multiple aspects of landscape-scale modelling (*e.g.*, processes, data, scales) and the corresponding multiple disciplines involved establish an inherent 'real-world' complexity. The model has to manage this complexity with the ultimate goal to provide (or support) a basis for regulatory RA and RM decision-making. The need for a structured model was reflected by the need for structured model development. This justified an excursion into software development methodology.

5.2 Software Development Methodology

5.2.1 Summary

The development of a model is to a considerable extent a software development effort. The craftsmanship of software development, however, is rarely a core skill of natural scientists. In order to narrow the gap between the available and required experience and skills needed to build a landscape-scale model, roles in software development and software development activities (*e.g.*, requirements analysis, architecture, system design, implementation) were employed and adapted from software development methodology. This structuring process was found to be of particular importance as the present model development activities were done by only a few persons.

The development process was divided into five major parts: (i) The identification of the model context together with stakeholders defined the model 'environment' and business goals; (ii) the functional requirements to the model as well as the non-functional aspects were specified; (iii) concepts were developed (including the software architecture) according to the range of requirements, and considering different perspectives of software development; (iv) in the system design step the technical solutions were defined and (v) subsequently implemented into software code (Figure 8, Section 5.2.2).

These parts were considered repeatedly in an iterative ('Agile') process. Agile software development methods were identified to fulfil the demand for a structured and managed development while maintaining flexibility and adaptability, both which is necessary for an innovative model development process.

Iterations were employed for the entire project as well as for its numerous sub-projects. Each iteration comprised all activities of the development process and was accompanied by extensive communication. In doing so, experiences obtained at each step could immediately influence subsequent steps, and hence, kept the development process adaptive.

For a scientific model development, the role of a software architect revealed valuable. The architect takes a central and active role in the entire process activities, *i.e.*, from the business analysis over system design and its implementation up to software testing and its use. In this range, the software architect has a key responsibility in the development of the software architecture and has to take different viewpoints.

The general requirements of the Xplicit development were derived in the evaluations of the regulatory framework of PPPs and the necessity for improved landscape-scale context in risk characterisation, RA and RM (Part 1, Section 4). These general requirements were evaluated in detail and were translated into system architecture and design.

The business analysis builds the entry point of software development. It contains the detailed analysis and description of the problem and general goals from the business view. In the Xplicit development, this step comprised communication with experts of different institutions and stakeholders involved in RA and RM of PPPs (*e.g.*, authorities, research, Section 4.5.1, scientific community, *e.g.*, SETAC, Schad 2009, Schad *et al.* 2011, Schad & Schulz 2011).

In the business analysis three different levels were considered: The business level asked "*what is the added value of the model?*"; the user level took the user perspective of the model (different user groups were distinguished); the system level evaluated requirements on system design (*e.g.*, modularity) and took also the technical perspective.

The development of the Xplicit software architecture was guided by adapted views of the 'Architecture Cube' (Schäfer 2010) which structures architecture in three dimensions. From the variety of guiding principles for software architecture, 'Modularity', 'Consistency' and 'Separation of Concern' were of particular importance in the Xplicit development. Software architecture has evolved standardised solutions for recurring problems, called 'Pattern'; *e.g.*, 'Layering', 'Mediator', and 'Service-Oriented Architecture' (SOA). The implementation of the Xplicit modelling framework followed an Object-Oriented-Programming (OOP) design and was done using the Microsoft .NET Framework and the C# programming language. Software testing (*e.g.*, Unit-/System-Tests), model verification and validation were distinguished.

5.2.2 Development Process and Roles

The development of a mathematical model for landscape-scale risk characterisation has to deal with different types of complexity (*e.g.*, scientific and technical complexity, regulatory framework, Section 4), with innovative elements and with the usual project constraints regarding resources. This requires, in a first step, to define an appropriate development process with related roles.

Software development methods were adapted from Schäfer 2010, Pilone & Miles 2008, msdn.microsoft.com, different books on the Microsoft Azure platform (Jennings 2009, Krishnan 2010, Sirtl 2010, Hay & Prince 2011), C# books (*e.g.*, Louis *et al.* 2010), articles in Wikipedia.org, and further sources (noticed in corresponding text passages). The adapted methods are regarded as a valuable 'by-product' of this thesis, as they can serve as a template for comparable projects of scientific model development in a commercial environment ('Agile scientific-informatics – partnership').

5.2.2.1 Basic Development Process

Five major activities structured the development process (Figure 8):

i. Business objectives: Identification of the model 'environment', together with stakeholders and definition of the model business objectives (Section 4.5).
ii. Requirements: Efficient specification of the functional requirements as well as the non-functional aspects of the model. Specifications need to be adaptable according to the experiences gained in the course of the development process.
iii. Concepts: The development of model concepts and software architecture according to the identified requirements. Different perspectives should be taken into account in the development of the model architecture (Section 5.2.4) without referring to a technical solution.
iv. System design: Definition of the technical solutions ('design') to realise the model architecture, taking up-to-date technology and tools (*e.g.*, Section 5.2.4.4 and 5.2.4.5) as well as non-functional requirements into account. The description should be as detailed as necessary to allow unambiguous implementation according to the business goals.
v. Implementation: Turning the system into software code. Again, non-functional requirements are to be taken into account.

These major development activities were processed iteratively ('Agile Development', Section 5.2.2.3). Iterations were employed for the entire project as well as its numerous sub-projects. Each iteration defined clear targets and comprised all activities. This allowed to immediately introducing experiences obtained at any step which assured an adaptive development process.

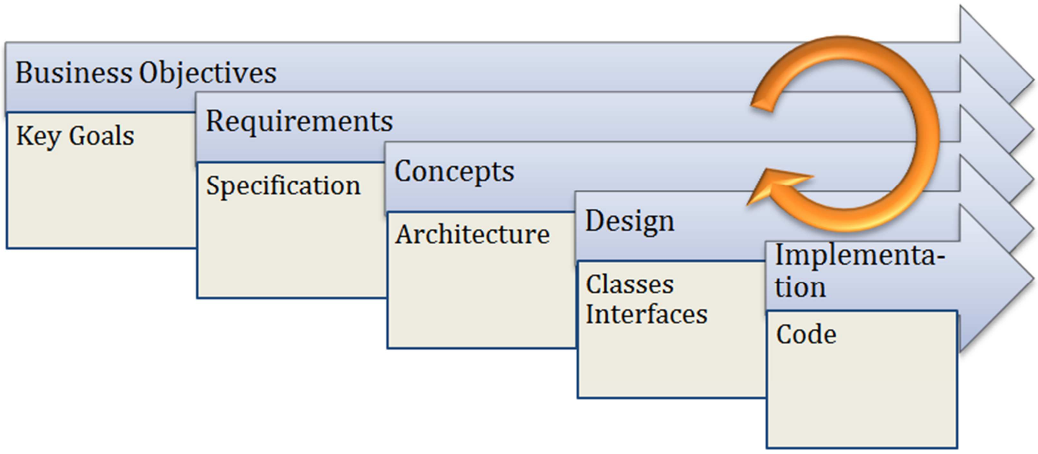


Figure 8: Major Xplicit development activities (adapted from Schäfer 2010) as a sequence of defined steps from the evaluation of the business objectives to implementation. In fact, all steps can basically run in parallel and are subject to iterations (cycle) to ensure an adaptive process. The sequence was applied to the whole project and its sub-projects.

5.2.2.2 Roles

Software development methodology explicitly defines different roles, comprising, *e.g.*, the project leader, the business analyst, the system designer, and the programmer. In recent years, the role of a software architect has become prominent (Schäfer 2010). In a sense, the architect acts as an agent between the different roles over the entire development project, but also has to design and sketch the system. The architect develops a solution to the problem (business requirements and aspects, Section 5.2.3) with focus on the fundamental elements. Ideally, skills of an architect range from understanding the business objectives, over system design and technological aspects, down to programming (besides soft-skills of a project manager).

The software architect role was adapted to the present model development with its numerous scientific, regulatory and engineering facets. In the course of the development, the roles of project management, architect and programmer were sharpened. The architect was responsible for business and requirements analysis (in different architectural dimensions, Section 5.2.4), and developed concepts and system design, whereas the programmer did the implementation, with a broad overlap of the roles in system design (Figure 8).

Despite the necessity to define clear roles, active cooperation, communication and flexibility of people who take these roles are major success factors to a development project with innovative characteristics that is organized using the described adaptive development process (Figure 8, Section 5.2.2.1).

5.2.2.3 Agile Development

The general requirements to a landscape-scale model for ecological risk characterisation comprised a number of facets and indicated an inherent complexity (Section 4.5). It seems clear that the development steps shown in Section 5.2.2.1 (Figure 8) could hardly be processed once for the entire project or its sub-projects without any feedback from later steps.

The innovative nature of the project required to apply a structured, yet, adaptive development method. Knowledge and experiences gained at any step in the course of the development process could be crucial to other steps. Thus, a clearly managed but iterative development method was needed.

The required adaptivity, structure and effectiveness were found to be best represented in Agile Software Development (*e.g.*, Schäfer 2010). Wikipedia.org:

"***Agile software development*** *is a group of software development methodologies based on iterative and incremental development, where requirements and solutions evolve through collaboration between self-organizing, cross-functional teams. It promotes adaptive planning, evolutionary development and delivery; time boxed iterative approach and encourages rapid and flexible response to change. It is a conceptual framework that promotes foreseen interactions throughout the development cycle.*"

Iterations are a major element of Agile Development (Figure 9). The following characteristics of iterations were adapted in the Xplicit development:

- Basically, in each iteration all development activities are carried out (Figure 8, Section 5.2.1). Iterations can be seen as a sequence of self-contained project cycles, and hence, represent 'mini-projects'. Thus, iterations are planned and defined by their goals and timeframe and define a clearly structured (short) development cycle.
- Communication and close interaction is key to Agile Development, and hence, regular part in iterations. Typically, phone and Web-conferencing happened twice a week ('Stand-up meetings', *e.g.*, Pilone & Miles 2008).
- In iterations, documentation along the development process, from business analysis to implementation, was done at a minimum. Competence, soft-skills and responsibility of the contributing people were weighted more than formalities.
- Planning of iterations comprised keeping track of the 'Burn-down' status (*e.g.*, Pilone & Miles 2008).
- Activity focus in iterations along the development steps depended on the project phase (Figure 9, Figure 8). In early phases, an iteration emphasised more on business analysis, requirements development and architecture. Yet, this was typically accompanied by work on system design, and prototype implementations in order to *e.g.*, test different options or check possible dead ends. At later stages, focus was moved to implementation and testing, yet, requirements development and system design were still reconsidered and adapted if necessary.

- Typical duration of iterations was days to weeks. A manageable number of iterations (of different sub-projects) ran in parallel. While some sub-projects were in the requirements or early conceptual phase, others were implemented or tested.
- Iterations enable stepwise refinement and extension, and hence, allow for 'non-perfect solutions' (regarding functionality criteria, not quality aspects). This minimises the risk of failure in achieving the major project goals (business requirements).
- Unit-Tests, *i.e.*, testing code units by the programmer (*e.g.*, methods, classes) were part of iterations. System-Tests, *i.e.*, testing the system as a whole from outside were intensified at later development phases (Figure 9).
- Iterations comprised refactory, *i.e.*, cleaning and optimising code without changing its visible functionality.
- A repository (Tortoise-SVN, tortoisesvn.net) was used to store and provide the latest 'Build', *i.e.*, a running version, centrally.
- Example iterations in the Xplicit development: The requirement for scalability requested for parallel processing. The ultimate design and implementation of the distributed computing approach (Section 5.3.4.14) evolved in iterations of different hierarchically organised sub-projects. Early iterations identified a queuing system in preference to a centralised one. Later iterations sharpened the communication of the *Xplicit-Processors* (Section 5.3.4.3).

<u>Driving Factors</u> (Schäfer 2010) that affected the adaptation of architecture and implementation in iterations were, *e.g.*, the risk of failure as not to result in a model that fulfils the requirements, risk characterisation Use-Cases (*e.g.*, Pilone & Miles 2008), particular model features (*e.g.*, scale dependency) and the risk of faulty calculations with severe effects to RA and RM.

<u>Software development phases</u> (Figure 9) represent the sequential stages of a software development (sub-) project. In the 'Inception' phase, the problem is evaluated and a first proposal to its solution is derived. The 'Elaboration' phase results in a viable architecture that clearly states what has to be achieved during development, based on a business analysis. In the 'Construction' phase, an applicable beta-version is being implemented (typically consuming most resources) and including Unit-tests. The 'Transition' phase leads to the product as requested by the business requirements comprising documentation and user training (Schäfer 2010, adapted).

Figure 9 illustrates the relationship between development phases, activities (Figure 8, Section 5.2.1) and iterations. The illustration shows that basically all activities contribute to the different phases, yet, with different weights.

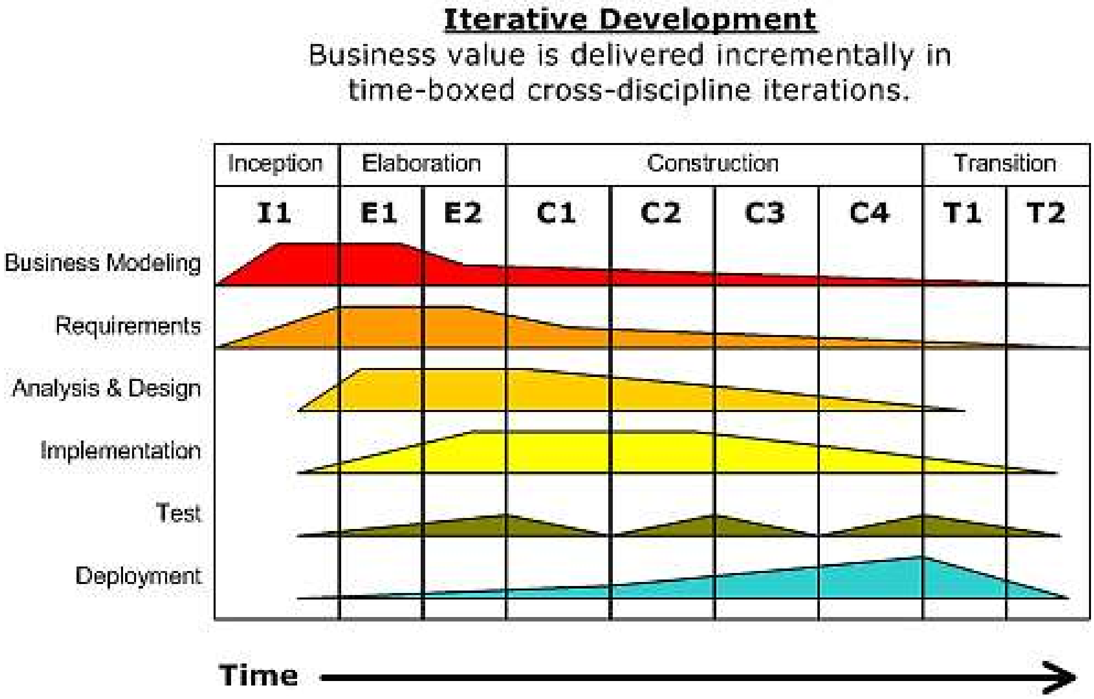


Figure 9: Relationship between software development phases (columns), activities (rows) with their resource intensity (coloured graphs), and iterations ('I1, E1, E2, …, T2') (Wikipedia.org, 'Unified Process', Development-iterative.gif).

5.2.3 Requirements Analysis

The general requirements of the Xplicit development were derived in the evaluation of the regulatory framework of PPPs and the resulting necessity for improved landscape-scale context in risk characterisation, RA and RM (Part 1, Section 4). These general requirements were evaluated in detail and were translated into system architecture and design.

The business analysis builds the entry point of software development. It contains the detailed analysis and description of the problem and general goals from the business view. In the Xplicit development, this step comprised communication with experts of different institutions and stakeholders involved in RA and RM of PPPs (*e.g.*, authorities, research, Section 4.5.1, scientific community, *e.g.*, SETAC 2013a, Schad 2009, Schad *et al.* 2011, Schad & Schulz 2011).

The business analysis leads to functional and non-functional requirements. Schäfer (2010) considered three different levels to assess business requirements:

- The business level asks "*what is the added value of the model?*", which was specified to "*what does the model contribute to improve ERA and RM?*". The business level defines the context of the development (Figure 5) and considers the effort from its ultimate goals.
- The user level takes the user perspective of the model. Three different user groups were distinguished: (i) the modeller who *applies* a predefined '*Xplicit-Model*' (Section 5.4) by parameterisation, (ii) the '*Xplicit-Model*' builder who derives an applicable model from

the *Xplicit-Framework* (Section 5.3), and (iii) the *Xplicit-Framework* developer who is able to extent the framework by adding code.

- The system level evaluates requirements on system design (*e.g.*, modularity, scalability, data, processing cost) and takes also the technical perspective (*e.g.*, platform).

Procedures employed in requirements analysis were adapted from Schäfer (2010), Pilone & Miles (2008) and Wikipedia.org ('Requirements analysis').

Key aspects and their sequence considered in requirements analysis are summarised in Figure 10. In an initial 'Framing' step, the context and its effect on model design was evaluated and described. In the analysis step, goals were prioritised and translated into tentative drafts. The documentation fixes the functional and non-functional requirements. The Validation describes criteria and a means to review the model.

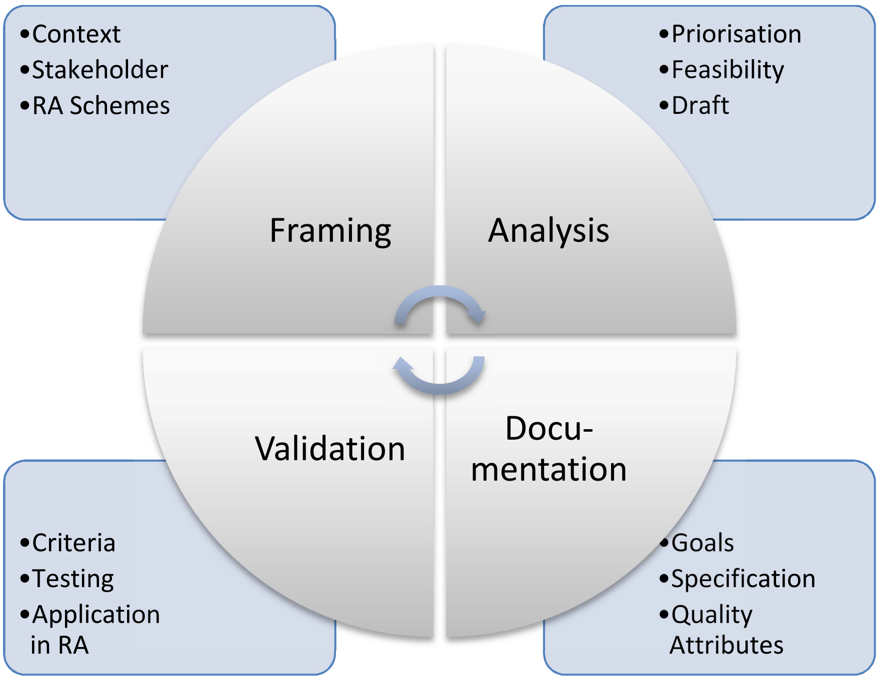


Figure 10: Requirements analysis (Schäfer 2010, adapted).

This structure was applied effectively within the Agile development methods (Section 5.2.2), in which requirements analysis was iteratively employed.

Further techniques used to evaluate requirements:

- Use-cases describe steps in an interaction between 'actors' (human or external system) and the system in focus to achieve a certain goal. Use-cases supported the definition of detailed functional specifications and user operations (*e.g.*, configuration, evaluation of the simulation outcome). In Agile development iterations, Use-cases were mostly described briefly and used in team discussions.

- Scenarios were used to describe envisaged conditions for the application of the model (or its components). Scenarios built an important means to specify the system behaviour. For example, the range of RA problems to be processed by the model resulted in requirements for a generic approach of a core functionality, yet, adaptable to specific RA problems.

Quality Attributes define fundamental requirements (implicitly) expected from a software in addition to business functionality. The analysis of Quality Attributes was split into three groups (Schäfer 2010, adapted): capacity (performance, scalability), applicability (availability, usability, security) and administration (customisation, verification, maintenance).

5.2.4 Architecture

5.2.4.1 Architecture Dimensions

The development of the Xplicit software architecture was guided by the views of the 'Architecture Cube' (Schäfer 2010). There, architecture is structured in three dimensions, each of which consisting of three traits (Figure 11, Table 4).

A 'Layer' represents an abstraction of a problem, a 'Viewpoint' differentiates how we look at the system, and the 'Perspective' models an aspect corresponding to the three perceptions in the Unified Modelling Language ('Structure', 'Behaviour', 'Interaction'). With the aim to structure the Xplicit architecture development, the static 'Perspective', *i.e.*, describing the static elements of a system, was mainly employed. The remaining dimensions correspond to the front of the 'Architecture Cube' which is called the 'Architecture Matrix', Figure 11).

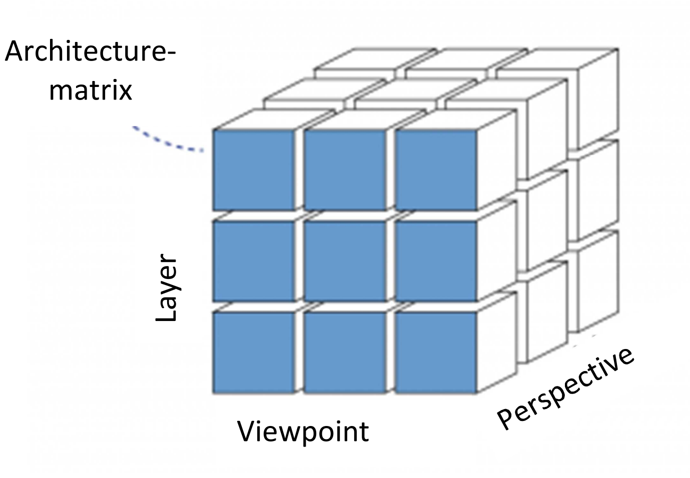


Figure 11: 'Architecture Cube' with the three dimensions 'Layer', 'Viewpoint' and 'Perspective'. The blue coloured front of the cube represents the 'Architecture Matrix' (Schäfer 2010).

Table 4: Views to software architecture taken from different dimensions of the 'Architecture Cube' (Schäfer 2010, adapted).

Dimension	Trait	View
Layer	Business	View from business goals as the ultimate purposes of the system; added value of the model to business.
	System	View from the IT system (*e.g.*, model components, modules).
	Technology	View from technological elements (*e.g.*, platforms, databases, protocols).
Viewpoint	Conceptual	View from problem abstraction, underlying ideas, theoretical building blocks.
	Operation	View from using the system (model) in the intended context, including, *e.g.*, its temporal behaviour and interaction.
	Implementation	View from code organisation, classes, methods, interfaces and modules.
Perspective	Structure	View at the static structure of the systems entities (*e.g.*, components, classes, modules).
	Behaviour	View at dynamic behaviour of entities.
	Interaction	View at interaction of entities, data and information flow.

5.2.4.2 Guiding Principles

An overarching guiding principle in scientific modelling is attributed to Albert Einstein, called 'Einstein's Constraint': "*Everything should be kept as simple as possible, but no simpler.*" (Wikipedia.org). This expression well represented the challenge of a landscape-scale model for ecological risk characterisation to deal with the real-world complexity (represented by landscape-scale entities and processes) on the one hand, and to aggregate its results into rather simple statements in order to support the RM decision-making process on the other.

Besides simplicity, software architecture has developed a fundus of guiding principles of which some were adapted to the Xplicit development (Schäfer 2010, Table 5).

Table 5 Guiding principles in software architecture applied in Xplicit development (adapted from Schäfer 2010).

Principle	**Use in Xplicit Architecture**
Modularity	• Key principle to manage complexity. Conceptual, functional or technical building blocks were defined at different system levels. • Modular design from (i) 'top-down' and (ii) 'bottom-up' view. (i) view from system's top-level; breaking the system stepwise into modules which can independently operate; (ii) view from small system parts; combination of parts to modules.
Consistency	• Consistent concepts at different system levels (*e.g.*, higher-level components and modules, lower-level entity management and interfaces to external models).
Abstraction	• Reduction of the range of RA problems to their main aspects and definition of a generic design. • Representation of real-world entities as model objects.
Separation of Concern	• A guiding principle that related to 'Modularity', yet, was considered in the design down to lower-levels (*e.g.*, classes, methods) in order to minimise the distribution of functionality across model entities.
Secrecy	• 'Information hiding' was considered as a major principle of object oriented software. Thus, entities make only public what is necessary to their functionality.
Flexibility	• Flexibility was related to 'Abstraction' in a sense that the model should have a core functionality (low flexibility), yet, which should be designed to be adaptable to specific RA problems (high flexibility). • Model adaptability concerned also envisaged developments in RA (*e.g.*, use of mechanistic population models, Section 5.3.5.7).

5.2.4.3 Aspects

The term 'Aspect' is used for non-functional requirements to software development. "*An aspect of a program is a feature that is linked to many parts of a program, but which is not necessarily the primary function of the program*", (Wikipedia.org).

The evaluation of aspects was guided by the 'Architecture Matrix' (Section 5.2.4.1, Figure 11). Stakeholders and the model context contributed to non-functional requirements (Section 4.5). Major aspects considered in the evaluation comprised, *e.g.*, applicability, data processing, ergonomics, maintenance and business rules.

5.2.4.4 Pattern

Software architecture has evolved standardised solutions for recurring problems, called 'Pattern'. The following 'Pattern' were employed in the Xplicit architecture:

- 'Layering' is one of the common pattern used, *e.g.*, in computer communication. A layer physically depends only on underneath layers. 'Layering' was used *e.g.*, to separate configuration, control, business logic, and data access.
- 'Adapters' play an important role in the design of the framework as they link external models to the framework (*Xplicit-Framework*, *Associated-Models*, Section 5.3.4.10). An adapter can be regarded as a translator of the 'foreign' interface of an external model to a known interface of the *Xplicit-Framework*.
- 'Composites' of homogeneous objects; *e.g.*, Xplicit makes use of collections of objects of the same type (*e.g.,* list of receptors).
- 'Mediators' as central instances ('hubs') that mediate the interaction of objects; *e.g.*, managements of model entities (*e.g.*, `ReceptorManagement`, Section 5.3.4.8) or distributed computing (Section 5.3.4.14).
- 'Abstract classes' in Object-Oriented-Programming (OOP).
- Service-Oriented Architecture (SOA, Section 5.2.4.5).

The Xplicit architecture was also influenced by technology availability and their conceptual and technical solutions to typical problems ('Artefacts'): *e.g.*, Oracle (RDBMS, Relational Database Management System), XML, Microsoft Azure (Microsoft 2013, *e.g.*, distributed computing, message queues, shared counter), Microsoft .NET Framework (C# language).

5.2.4.5 Service-Oriented Architecture

Landscape-scale risk characterisation involves multiple disciplines (Section 4.4 and 4.5), *e.g.*, exposure, eFate and effect modelling, as well as geodata processing.

Dividing the multidisciplinary problem into units which offer a specific thematic and/or functional service was regarded as a rational step to manage complexity. At the same time, distinct service units with clear agreements (contracts, interfaces) about their characteristics and availability can contribute to the harmonisation of higher-tier risk characterisation, and hence, to support the development of landscape-scale risk characterisation, RA and RM in the future.

Ravi Subramaniam introduced Service-Oriented Architecture (SOA) as follows (2008, IBM, Figure 12): "… Figure 12 *depicts the layers of an SOA solution. End users (…) use business applications, which can be rich-client, mobile, portlet-based, or Web-based to invoke business processes. A business process is created by the composition and choreography of business services provided by service components. Service components may interact with other operational or legacy systems within the enterprise to acquire the requested information or perform a business task. Services are at the heart of this multilayer architecture and are components that realize service flows and processes. There's a notion of a service consumer and a service provider. Integration (…), a security and monitoring infrastructure, data architecture,* *and governance are depicted as foundational layers of capability underpinning an SOA solution*."

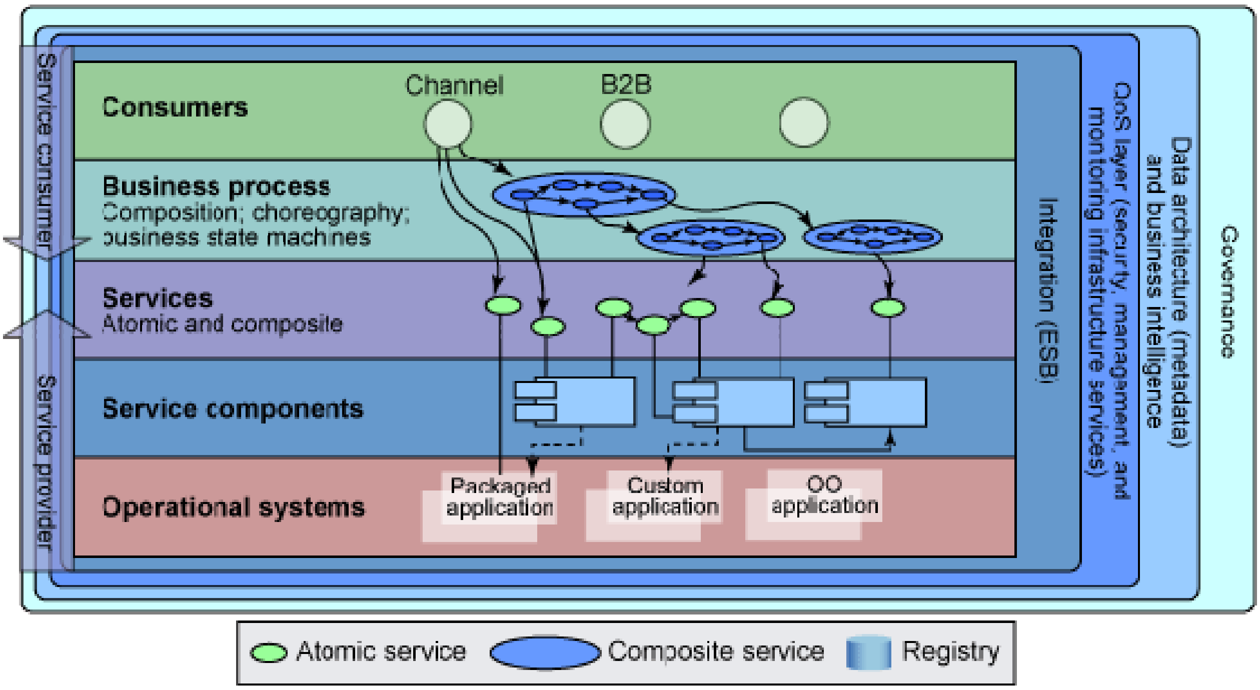


Figure 12: Layers of an SOA solution (IBM 2008).

The SOA idea to "*build architectures on the basis of interfaces and their implementation… where… the interface represents a full business-service* (Schäfer 2010)" had a substantial influence on the Xplicit architecture. SOA can be seen as a 'Pattern' (Section 5.2.4.4).

The identification of potential SOA components was done in combining 'bottom-up' (*i.e.*, by evaluating modules in order to cluster them into services) and 'top-down' (*i.e.*, from the business goals, by partitioning the business process into independent system components).

One of the most obvious components of a landscape-scale model approach that can be regarded as a service component is the processing and provision of geodata. Actual process modelling (*e.g.*, exposure, eFate and effect modelling) was intended to be separated from geodata processing which was regarded as a SOA component (*e.g.*, *LM3*, *Xplicit-Distance*, Section 5.3.5.2 and 5.3.5.6). Furthermore, recurrent data processing was conceptually considered as SOA components (*e.g.*, aggregation and evaluation of Xplicit simulation outcome using SQL and R-Statistics, Section 5.3.4.4).

A complex system like a landscape-scale risk characterisation model can be built as a SOA solution (Figure 12) with SOA components comprising all dividable components (*e.g.*, geodata providers and processors, agricultural cultivation practice models, exposure and eFate models, population models, data analysis, etc.). Although the multiple Xplicit software components have not been realised in a SOA, the idea was reflected in building the Xplicit architecture and the resulting modular system design. Basically, modules can be turned into SOA components.

5.2.5 System Design

System design defines the technical solutions ('design') as a realisation of the model architecture (Section 5.2.4). As the model was intended to take a 'look ahead' with respect to potential future landscape-scale risk characterisation, RA and RM (Section 4), up-to-date technology and tools should be taken into account (*e.g.*, Section 5.2.4.4 and 5.2.4.5). However, the realisation of these goals in the course of this thesis had to be balanced against resource limitations. Thus, the governing design principle was to give technological guidance on the future technological orientation of the system while building a model that could be applied immediately by using available technologies (*e.g.*, RDBMS). Beside the realisation of the software architecture, system design had to take non-functional requirements into account.

The development of the system design followed Agile processes (5.2.2) and profited from experiences made with a previous version (Schad & Schulz 2011). The Xplicit system design is summarised in Section 5.3.4.

5.2.6 Implementation

Following Agile software development processes (5.2.2), implementation was done in close communication between the software architect and the programmer. As the project matured, and within iterations, both roles developed a broad overlap in sharpening the system design. In iterations, coding of a unit (*e.g.*, class, module) was discussed by taking an outside standpoint, *i.e.*, defining what the code was expected to do. This method was adapted from the 'Design by Contract' approach (Schäfer 2010) which sees the functionality that a unit has to provide as a contract between the user of that unit (code) and the code.

Implementation of the Xplicit modelling framework followed Object-Oriented-Programming (OOP). Implementation was done using the Microsoft .NET Framework (using release 4.0, Microsoft 2012b), the Microsoft C# programming language and the Microsoft Visual Studio integrated development environment (Professional and Ultimate, Version 2008 and 2010). Thus, Xplicit models runs on platforms at which Microsoft .NET Framework is running, which applies primarily to MS Windows® Operating Systems (XP, Windows 7, Server 2003 and 2008, Microsoft 2013). However, according to the information of the Mono project (*"An open source, cross-platform, implementation of C# and the CLR that is binary compatible with Microsoft.NET*", Xamarin 2012), Xplicit should be executable on further operating systems, *e.g.*, Linux or Unix.

In iterations, the code was subject to refactoring. Refactoring comprised code simplification, cleaning of non-used code parts, etc., without altering code functionality as perceived from outside a code unit. Refactoring efforts concerned, *e.g.*, the optimisation of data structures, the improvement of processing speed and the reduction of memory consumption.

The software versioning and revision control system Apache Subversion was used (subversion.apache.org), together with the client Tortoise-SVN (tortoisesvn.net) to manage the source code and to document versions.

5.2.7 Documentation

Following Agile software development methods (Section 5.2.2), documentation during the development process was minimised to cost and operationally effective levels (*e.g.*, requirements specification, architecture, system design, project management). Documents were formatted to have a clear purpose and a focus on the needs of the addressee.

Documentation of the resulting *Xplicit-Framework* was done at three levels:

1. Code comments:
    a. Common code comments ("//") to explain *why* a specific code design was chosen.
    b. XML comments ("///"), to build documentation directly from the Visual Studio .NET source files. The slashes tell a parser that the marked parts represent an XML comment. The C# parser extracts the XML comments and writes them into an XML file for further processing, *e.g.*, to generate help files (below).
2. User and developer manual were represented by a Microsoft help file ('chm' – file) which was generated from XML comments and extended by manually added conceptual text.
3. This thesis documents the project motivation, background and context, and summarises the architecture and design of Xplicit, as well as its example use in regulatory RA.

5.2.8 Tests

Software testing (software validation), model verification and validation were distinguished.

Software testing primarily regards the software as a technical system and was focused to test software elements: Unit-Tests (or 'White-Box-Tests', Pilone & Miles 2008) were conducted at different software units (*e.g.*, methods, classes, modules) and were parts of iterations (Section 5.2.2). Unit-Tests refer to code unit testings by the programmer (developer) who has good knowledge of the software details. In practice, 'White-Box' testing was done in seamless transition to 'Grey-Box-Tests' (Pilone & Miles 2008). This built the main testing level with respect to the *Xplicit-Framework* (Section 5.3). As the framework as such does not represent an immediately applicable model, it fulfils only a subset of the requirements (Section 5.2.3, 5.3.2). Therefore, System-Tests, *i.e.*, testing the entire system as a whole from outside ('Black-Box-Tests', Pilone & Miles 2008) were mainly reserved to *Xplicit-Models* (Section 5.4).

Verification of a model requires to view the software system as a whole. The system was verified against the range of functional and non-functional requirements (Section 5.2.3, 5.3.2), including technical aspects. Verification does not refer to the usefulness of the model with respect to address regulatory RA problems. Verification builds on a statistical certainty, as system testing cannot assure that the model is 100% error-free. Case studies shown in Part 3 (Section 6) have contributed to System-Tests, hence, *Xplicit-Model* verification. Georeferencing of model outcome using GIS supported model verification ('visual debugging'). A status of an *Xplicit-Model* being 'verified' can hardly be achieved (Macal 2005), but a status of 'having passed certain verification tests'.

System-Tests ('Black-Box-Tests', Pilone & Miles 2008) can also be applied to external models which are linked to the *Xplicit-Framework* (*Associated-Models* and *–Services*, Section 5.3.5) as they represent standalone model approaches (*e.g.*, Schad & Gao spray-drift model, Section 5.3.5.4; geodata providing service, Section 5.3.5.2).

Model validation has to be regarded in context to its purpose in a RA and RM problem formulation, hence, in context to the scenario within which it is employed (*Xplicit-Model-Scenario*, Section 5.4). The straightforward question of whether the model correctly represent (or reproduces) the behaviours of the modelled real world system can hardly be answered, as the model is a drastic simplification of the real-world system. A model scenario is typically based on available experience and data (*e.g.*, environmental and agricultural conditions). Variability and uncertainty of the landscape-scale factors led to the use of probabilistic methods. The comparison of the model (scenario) outcome to real-world conditions requires considerable spatiotemporal sampling densities in practice.

For these reasons, the question of validation needs to be specified in context of the model purpose. The ultimate goal of model validation is to assess the model's (and scenario's) usefulness in addressing the RA and RM problem formulation. Therefore, model validation can be regarded in the spirit of the well-known statement of George Box, "*Essentially,* a*ll models are wrong but some are useful*" (Box 1979).

In a RA and RM context, a useful model can be considered to support decision-making by reducing the overall uncertainty in the decision-making process (Bayesian view, Section 4.3.1.1), *i.e.*, as a contribution to improve the knowledge upon which improved RM decisions can be made. The model part in RM decision-making can range from informative, to supportive or even decisive. For example, in the RM question of where to invest windbreaks as a shelter of water bodies against spray-drift, a model can be used to characterise risk of water bodies at local scales (*e.g.*, case studies Section 6.3 and 6.4). In the ultimate RM decision, the outcome of the model can be directly implemented or can be regarded as a contributor to further available knowledge and expert judgement. Thus, a monitoring campaign intended to provide a basis for model validation need to be designed in correspondence to the actual model purposes.

5.3 The Xplicit–Framework

This section presents the *Xplicit-Framework* as developed in the course of this thesis. Ready-to-use models (*Xplicit-Models*), derived from the *Xplicit-Framework*, are presented in Section 5.4. For reasons of simplicity, the term 'Xplicit' is often used to represent the Xplicit modelling framework approach.

5.3.1 Summary

The development of requirements for a landscape-scale model for ecological risk characterisation resulted in a modelling framework (*Xplicit-Framework*) that consists of a modular core software which comprises the key business logic and covers operation flow with interfaces to external services and models. This framework provides the functionality for spatiotemporally explicit and probabilistic risk characterisation taking scale dependencies into account. From a software development view, in ecological risk characterisation, the *Xplicit-Framework* provides a 'Pattern' (Section 5.2.4.4) to derive models for specific RA problems (*Xplicit-Models*). This is done by configuring available components and by linking external models to the framework, *e.g.*, exposure, eFate or effect models for Non-Target-Organisms.

Xplicit-Models consist of four main components: A management component (*XM*), a frontend component (*XF*), a processing component (*XP*) and an assessment component (*XA*). The *XM* management component initialises a simulation, governs its processing and compiles its output. *XM* is configured via Extensible Markup Language (XML) that is prepared by using the *XF* frontend component and an XML editor. *XF* is accessible in different ways, *e.g.*, using a web browser. Individual simulation tasks are conducted by autonomous processing units (*XP*s) which operate in parallel in a distributed computing environment. *XM* and *XPs* build the *Xplicit-Engine* (*XE*), *i.e.*, the operative simulation unit. The *XA* component is used to analyse the compiled output of the *XE* and to report the results for risk characterisation, RA and RM.

An *Xplicit-Model* simulation comprises a series of different *Themes* (*e.g.*, cultivation practice, PPP use, exposure, eFate, effect) that are represented in the model by modules and are processed by *XP*s. The processing logic of a module is basically represented by external models (*Associated-Models*, *e.g.*, exposure or eFate models) that are linked to the internal framework core by adapters. Thus, *Associated-Models* have service characteristics and can be explicitly realised as service endpoints (which applies to some of the *Associated-Models* already implemented in the *Xplicit-Framework*, *e.g.*, geodata provision).

Xplicit entities (objects) are designed to represent natural entities, *e.g.*, farmers, fields, habitat segments (*i.e.*, abiotic receptors) or biotic receptors (representing biological entities and their attributes under assessment). Abiotic receptors can represent any habitat type (*e.g.*, terrestric or aquatic habitats) whereas biotic receptors can represent any Assessment Endpoint (*e.g.*, individual mortality, plant growth reduction, population abundance). This makes Xplicit generic, and hence, provides a consistent risk characterisation approach for RA problems of recurrent structures.

Xplicit simulations are conducted in time-steps that represent a discretisation of time as abiotic receptors represent the spatial discretisation of the landscape. Xplicit simulations, thus, manage the spatiotemporal state of model entities. Each time-step of the simulation, each of the *XPs* reports its state and *XM* combines these data into a spatiotemporal representation of the corresponding *Theme*. The compiled states can then serve as input for other modules or can be assessed by *XA*.

Variability (and uncertainty) are represented by PDFs and are processed using a Monte Carlo (MC) approach. The central paradigm of MC simulations (Section 4.5.5) is considered by resolving variability due to discretisation at local scales and by explicitly taking scale-dependencies into account. This is achieved within the *Xplicit-Framework* by assigning spatiotemporal units (*e.g.*, field, receptor, year, day) to the PDFs which are subject to MC sampling. The framework also provides the possibility to conducted nested MC simulations in order to perform uncertainty and sensitivity analysis (UASA).

The *Xplicit-Framework* is designed to be operational in a distributed computing environment and, thus, assures a wide range of scalability. Processing of resource intensive model objects (*e.g.*, landscape, *Themes*) can be done in small portions that are processed by *XPs* in parallel. In consequence, *Xplicit-Models* can be operated at a local Personal Computer, multiple servers in a network or at a cloud computing environment (Microsoft 2013).

Xplicit-Model complexity can be adapted to its purpose in a RA and RM problem. Thus, landscape-scale context (real-word factors, complexity) can be introduced stepwise.

5.3.2 Requirements

This section summarises requirements to the model functionality which built the basis for the model architecture and design. The basis for the requirement development was given by the general requirements (Section 4.5) as well as the underlying evaluations on regulatory RA and RM and the landscape-scale as a unit that provides the necessary context for refined risk characterisation of PPPs (Section 4).

5.3.2.1 Framing

The 'Framing' step built the entry point to the requirement development (Section 5.2.3, Figure 10) and aimed at describing the (direct) model context and its effect on model design (Table 6).

Table 6: Summary on Requirements analysis – Framing.

Subject	Framing Constituent
Context	• Regulatory RA and RM of PPPs (the general regulatory framework is described in Section 4.3.2 and is further evaluated in Section 4.5.1). • Further regulations affecting the use of PPPs, especially in view of future developments in crop production and risk characterisation (Section 4.3.3). • Regulatory research: *e.g.*, GeoPERA (Schad *et al.* 2006b, 2007), GeoRISK (UBA 2010), Schulz *et al.* (2007, 2009), LEMTOX (Thorbeck *et al.* 2009), ModeLink (SETAC Europe Technical Workshop, October 2012, April 2013).
Stakeholders	• Risk assessors and risk managers at authorities at European level (European Food Safety Authority (EFSA), European Commission and at Member States (*e.g.*, German Federal Environment Agency, UBA), as well as regional authorities. • PPP industry (*e.g.*, Bayer CropScience) with their experts (*e.g.*, modelling experts, safety managers, risk assessors, ecotoxicologists, regulatory experts, Information Technology (IT) departments). • Farmers, growers, beekeepers. • Scientific community (*e.g.*, SETAC 2013a, universities, institutions (*e.g.*, Julius Kühn Institut, JKI 2012)).
RA Schemes	• Risk characterisation, RA and RM schemes (Section 4.3.1), as defined in regulations (Section 4.3.2) and technical guidance documents (*e.g.*, EC 2002a, EC 2002b, EFSA 2012b, FOCUS 2001, 2007a, 2007b); tiered RA schemes with higher-tier option. Future developments in RA schemes (*e.g.*, EC 2012b). • EFSA scientific opinions (*e.g.*, EFSA 2010a, 2012a, 2012b), in particular the EFSA opinion on SPGs (EFSA 2010a), requesting improved explicit risk characterisation in different risk dimensions. • Practical experience from higher-tier RA at Member State level. • Exposure and eFate modelling (*e.g.*, FOCUS 2001, Rautmann *et al.* 2001). • Current developments in ecological modelling (Section 5.3.5.7, *e.g.*, ModeLink (SETAC Europe Technical Workshop, October 2012, April 2013)). • Risk communication (Section 4.3.1.4, *e.g.*, Streissel & Montforts 2010).

5.3.2.2 Analysis & Documentation

The general requirements to a landscape-scale model were developed in Section 4.5 and provided a preliminary prioritization for the (iterative) development of software requirements.

Feasibility of the developed requirements was assessed on the basis of the experience gained in the development and use of an earlier Xplicit version (Schad & Schulz 2011) and by implementation and testing of requirement subsets. This prototyping was done taking different views of the architecture matrix (Section 5.2.4) into account and affected the requirements for, *e.g.*, the model core, for its components and modules (*e.g.*, exposure, eFate, effect), as well as for its entities (*e.g.*, generic representation of habitat segments of Non-Target-Organisms). As part of the iterative development cycles, 'Prioritization', 'Feasibility', and 'Prototyping' were repeatedly conducted.

The documentation of requirements split into 'Goals', 'Specification' and description of the non-functional software 'Quality Attributes'. The following major 'Goals' of the model software development resulted from the iterations:

- Core model approach providing the key functionality (below) which is extendable by process models (and data) to define a specific landscape-scale model approach. Generic approach with respect to different habitats of Non-Target-Organisms.
- Core functionality for spatiotemporally explicit calculations of different processes including, *e.g.*, cultivation practice, exposure, eFate and effect calculation. Process calculations to be based on discretised landscape entities (using geodata). Ability to operate with external models, *e.g.*, exposure models.
- Consideration of variability and uncertainty of entities' properties by using a probabilistic (Monte Carlo) approach. The model should allow to assess the extent of an adverse effect and its probability to occur (*risk*, Section 4.3.1.1).
- Explicit consideration of scales by defining scales and scale-explicit operation, *e.g.*, for the use of PDFs and in the aggregation of results in order to allow risk characterisation at relevant scales.
- Adaptable, scale-dependent definition and aggregation of model outcome ('extent of an adverse effect') for risk characterisation. Basically, the result(s) of any process model should be able to serve as subject to risk characterisation (*e.g.*, exposure, effect) at different scales.
- Scalable processing to operate landscapes of different spatial extent.
- Modular, service-oriented model approach with the possibility to be extended by additional or more complex process models in the future.

The definition and (iterative) discussion of 'Goals' was accompanied by 'Use-cases' and 'Scenarios' (Section 5.2.3) which were taken from current and potential future RA and RM problems. The RA problem formulations given in the case studies of this thesis (Part 3, Section 6) provide an impression on current RA problems and the approach of stepwise introduction of landscape-scale context (*AutContext*, Section 4.2). For example, "*lower-tier (Tier-1) RA of Non-Target-Terrestrial Plants is protective, and so, does not allow for risk quantification. Refined risk* *characterisation was necessary by taking into account the variability of exposure and individual-level effects (dose-responses of 10 plant species and 7 assessment attributes). Quantification of effect extent was done for the three risk dimensions 'species', 'Assessment Endpoint' (AE) and 'space', at edge-of-the-field- and regional-scale.*" Two types of model *users* were distinguished to support the development of software requirements: Based on an available model core and external models (*e.g.*, for spray-drift calculation), (i) one user has to define and configure a specific model to address the RA problem ('*Xplicit-NTTP-Model*'), which is then employed by (ii) another user who is conducting the actual risk characterisation by parameterisation and running the '*Xplicit-NTTP-Model*'.

Documentation of 'Specifications' was also guided by principles of agile software development (Section 5.2.2.3), hence, 'Specifications' were discussed in detail and documents were limited to a necessary minimum. Some example higher-level aspects are summarised in Appendix 11.1 (Table A 1).

Besides functional requirements ('Specification', above), 'Quality Attributes' (QAs) refer to non-functional requirements and represent an important part of the requirements to the landscape model development, and hence, are likewise considered in the software architecture and system design. QA documentation was also guided by principles of agile development (Section 5.2.2.3). Some example higher-level aspects of QAs are shown in Appendix 11.1 (Table A 2).

5.3.2.3 Software Validation

Fulfilment of documented requirements was reviewed at the end of each developmental iteration (Section 5.2.2.3). Software validation criteria reflected the functional and non-functional requirements (Section 5.3.2.2) which were basically considered as measurable (*e.g.*, core functionality, cooperation with external models, geodata access, scale dependent PDF sampling using Monte Carlo, operation and idempotency of distributed computing). Testing was part of iterations and was conducted as described in Section 5.2.8.

Higher-level software validation concerned the model use in RA context which is discussed in Section 5.4.3.

5.3.3 Architecture

This and the next section (Section 5.3.4) summarise major aspects of the software (model) architecture and system design as they result from the software development process and the requirements described in Section 5.3.2. Software architecture and system design are delineated as representing different strata of abstraction (Eden & Kazman 2003). The 'Architecture' part (this section) introduces the high-level structure whereas the 'System Design' part (Section 5.3.4) provides a more detailed presentation of some major system elements. The section aims at introducing the Xplicit software, but does not claim to represent a formal software architecture and system description (*e.g.*, ISO/IEC 42010).

Software architecture is part of the software development process and describes the fundamental constitution of system elements and their basic interaction (Section 5.2.4). It can be seen as the transition of the requirements (Section 5.3.2) and principles (5.2.4) into system elements and structure, by predominately taking a global view on the system ("*The highest-level breakdown of a system into its parts*", MSDN, Microsoft 2012c). Changing the software architecture would require large efforts.

5.3.3.1 Software Framework

In their entirety, requirements for landscape-scale model for refined risk characterisation (Section 5.3.2) and, in particular, the request for a core functionality reflecting the key RA problem structure with the option to adapt this to specific RA problems, resulted in a software framework architecture referred to as the *Xplicit-Framework*.

The key characteristics of a 'Software Framework', which also apply to the *Xplicit-Framework*, can be summarised as follows (Wikipedia.org): "

1. ***Inversion of control*** *- In a framework, unlike in libraries or normal user applications, the overall program's flow of control is not dictated by the caller, but by the framework.*
2. ***Default behavior*** *- A framework has a default behavior. This default behavior must actually be some useful behavior and not a series of no-ops.*
3. ***Extensibility*** *- A framework can be extended by the user usually by selective overriding or specialized by user code providing specific functionality.*
4. ***Non-modifiable framework code*** *- The framework code, in general, is not allowed to be modified. Users can extend the framework, but not modify its code...*"

The *Xplicit-Framework* provides the core functionality of a (generic) spatiotemporally explicit and probabilistic landscape-scale model approach (Figure 13). External process models (*e.g.*, farmer activity, exposure, eFate, effect) are associated to this core in order to define ready-to-use models (*Xplicit-Models*, Section 5.4) for specific RA problems.

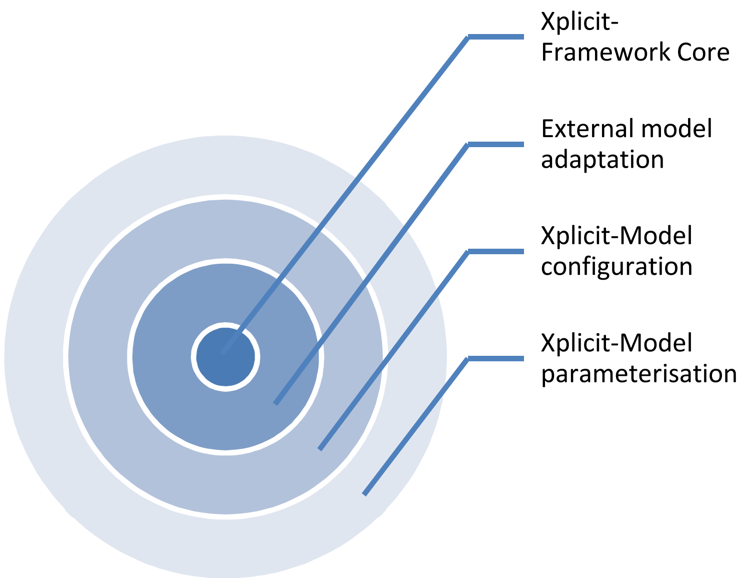


Figure 13: The *Xplicit-Framework* core and its relationship to specific *Xplicit-Models*.

The *Xplicit-Framework* provides the functionality according to the identified requirements (Section 5.3.2) including, *e.g.*, model configuration, management of model entities (*e.g.*, *Receptors*), simulation management (including initialisation, time-steps, simulation status), PDFs and Monte Carlo simulation (including a 2d-Monte Carlo approach), scale-dependent operation, processing of different *Themes* (*e.g.*, farmer activity, exposure, eFate, effect), distributed computing, post-processing, etc. Functionality is encapsulated in modules at different levels.

Major elements of the *Xplicit-Framework* architecture are (Figure 14, Sections 5.3.3.2 – 5.3.3.7):

- *Components* representing upper level (executable) modules providing the higher-level operation blocks with which the user gets in direct contact.
- *Themes* denoting actual simulation topics which are processed by (external) models. Each *Theme* is implemented as an independent module.
- *Entities* representing the key simulation objects: Farmers represent all cultivation activity (*e.g.*, cropping, PPP use); *Fields* are the farmers' activity targets and represent the primary source for PPP exposure; *Receptors* represent the fundamental unit-of-analysis of simulation processes and are operated in independent modules (abiotic *Receptors* represent habitat segments of Non-Target-Organisms, biotic *Receptors* represent Assessment Endpoints).
- Mathematical models describing the behaviour of natural systems or human activities (*e.g.*, farmer activity, exposure, eFate, effect). Models are encapsulated and thus provided by modules. External models are connected to the framework using adaptors.
- *Data Access* modules representing the technical access to external data sources and harmonise their representation in *Xplicit-Framework*-internal objects.

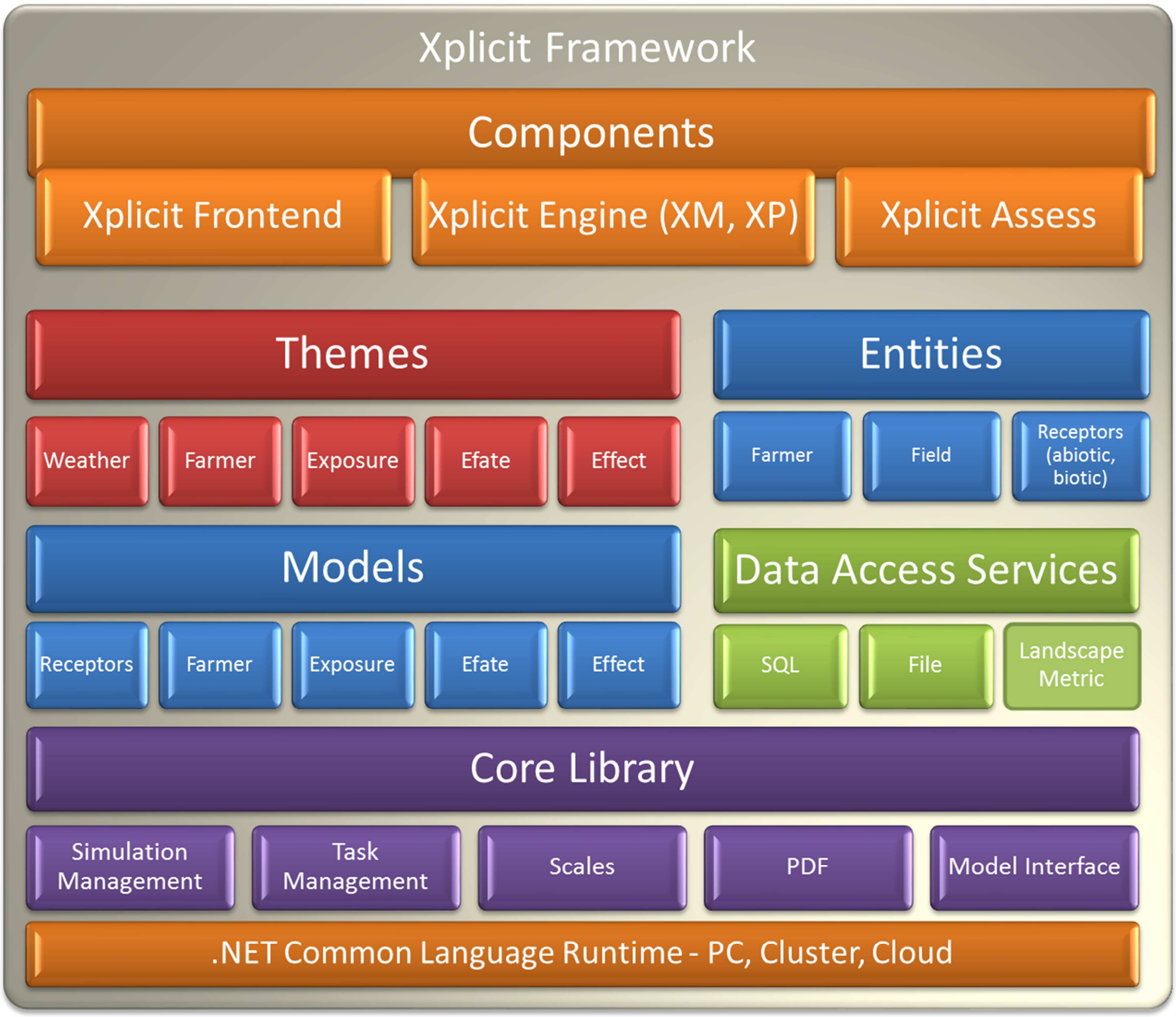


Figure 14: Elements of the *Xplicit-Framework* architecture (XM = *Xplicit-Management*, XP = *Xplicit-Processor*).

5.3.3.2 Components

Higher-level modularity concerns (i) configuration, (ii) simulation and (iii) evaluation. The corresponding modules are referred to as *Components* (Figure 15).

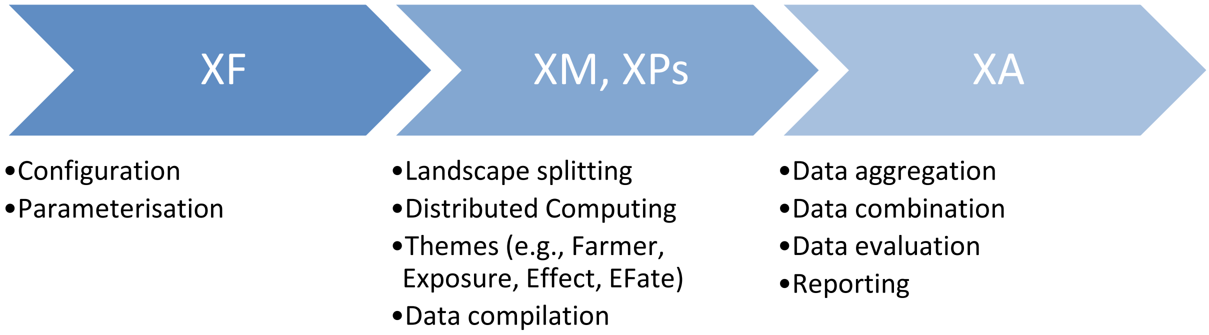


Figure 15: Xplicit *Components,* with simulation processing sequence (XF = *Xplicit-Frontend*, XM = *Xplicit-Management*, XPs = *Xplicit-Processors*, XA = *Xplicit-Assess*).

i. *Xplicit-Frontend* (*XF*): Configuration concerns both setting up an *Xplicit-Model* using the core capabilities of the *Xplicit-Framework* and the available modules (*e.g.*, geodata services, process models, etc.) and the configuration and parameterisation of existing *Xplicit-Models* (*e.g.*, PPP use, active substance DT50, dose-response, etc.). Configuration and parameterisation is conducted using an XML format that can be prepared and adapted by the XF component and by using generic XML editors. For user convenience, parts of this core XML configuration can point to further configuration sources (XML or plain text) which contain additional parameterisation options of the specific *Xplicit-Model.* The modularity of the Xplicit configuration and parameterization in combination with the use of an established and widespread format (XML) allows to set up Xplicit projects in different ways. Currently, the *Xplicit-Framework* provides a schema definition for preparing model configurations within XML editors and a web-browser user interface for parameterisation (using a web application for communication between *XF* and *XM* (below)). However, future versions of the *Xplicit-Framework* might provide additional interfaces (*e.g.*, an enhanced web-interface for configuration, a windows form or console application for parameterization, etc.).

ii. The *Xplicit-Management* (*XM*) and *Xplicit-Processors* (*XPs*) represent the actual processing *Components*. An Xplicit simulation comprises 1 *XM* and (typically) multiple *XPs*. *XM* receives an XML configuration (*e.g.*, XML file), splits, according to the configuration, the landscape into sub regions in order to generate work tasks that fit the proposed workload for parallel computing, prepares tasks for the processing units (*XPs*), administers the distributed computing and finalizes the simulation after completion. Actual model calculations are conducted by the *XPs*. An *XP* can physically reside at a computing unit in a network (*e.g.*, a local Personal Computer, a network server, in the cloud (*e.g.*, Microsoft 2013). It picks tasks from a task channel independently, performs the computational actions required by the task (which depend on the *Theme* associated with the task (*e.g.*, farmer activity, exposure, eFate, effect), the sub region of the landscape to which the task applies and the configuration of the model) and it reports the simulated outcome for each time step of the simulation to a result channel. After completing a task, an *XP* resets its state and starts listening the task channel for new tasks again, eventually picking the next task. The compilation of results in the result channel is performed by *XM*, which also writes the compiled results to a central data storage. As they represent the actual Xplicit simulation, *XM* + n *XP*s together are referred to as the *Xplicit-Engine* (*XE*).

iii. The outcome of an Xplicit simulation is evaluated by the *Xplicit-Assessment Component* (*XA*). The assessment process conducted by *XA* is thereby configured using XML. In *XA,* the *XE* outcome typically passes a 3-step evaluation (Figure 16): (i) In a 'Pre-processing' step, data reported by *XE Themes* are prepared for further assessment, (optionally) aggregated over risk dimensions (*e.g.*, maximum PEC(receptor) over simulation time) and centrally stored; (ii) using a data processing service, the results are processed in relation to the entire landscape data (*e.g.*, scale-dependent grouping of *Receptors*) to provide the basis for risk characterisation, which is (iii) concluded by a statistical analysis (including reporting and visualisation). Each sub-step of the *XA* evaluation process is internally represented by a processing module that is parameterized in the *XA* configuration.

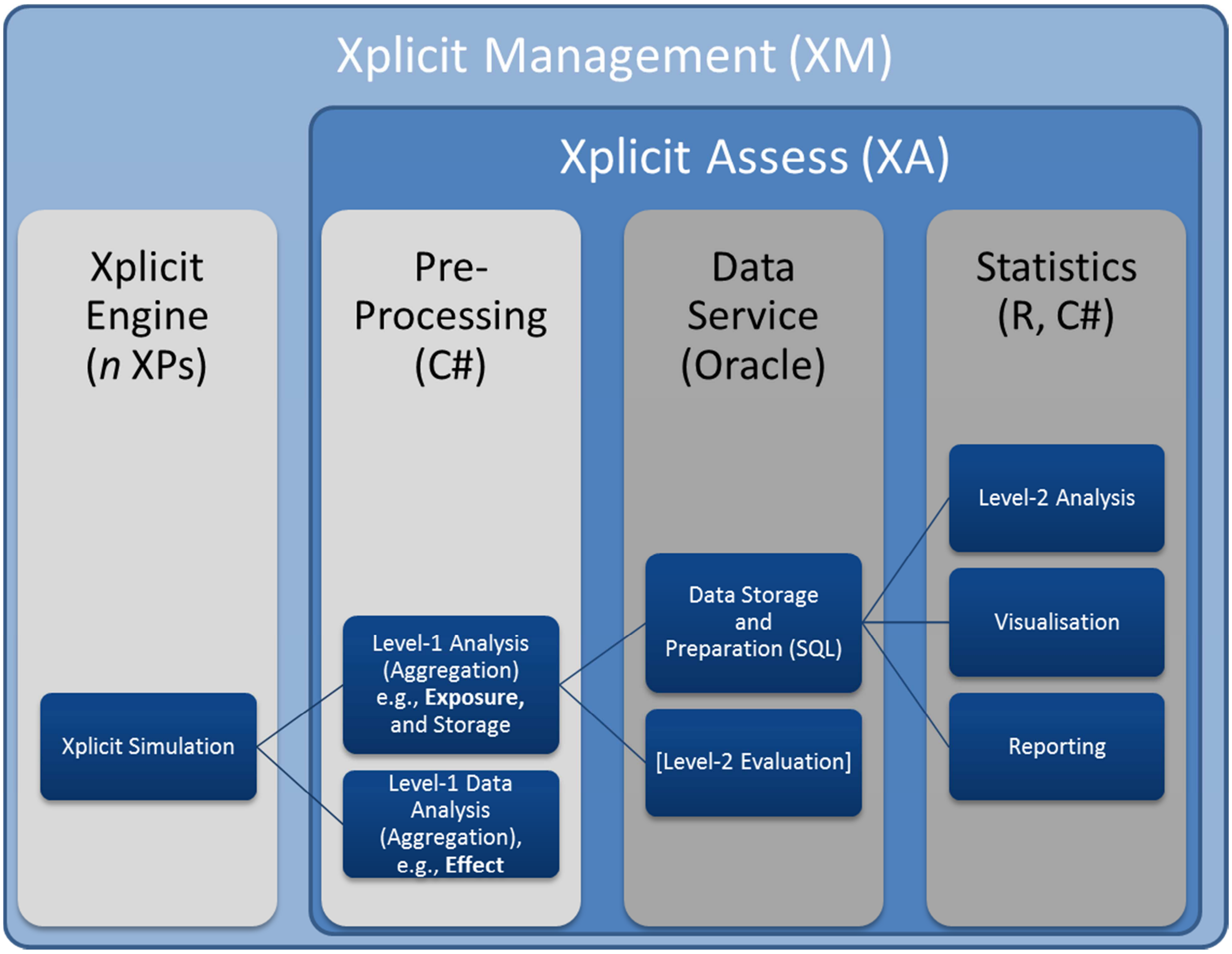


Figure 16: Evaluation of Xplicit simulation outcome in *Xplicit-Assessment* (*XA*) (steps in '[]' indicate optional steps).

5.3.3.3 Themes

The major Xplicit subjects are called *Themes*, that simulate actual study endpoints (*e.g.*, spatiotemporal distribution of substance concentrations (PECs) or ecotoxicological effects) or represent intermediate simulations targets like weather, farmer activity or substance reaching habitat segments (exposure of *Receptors*). *Themes* are processed in separate modules, which are typically linked to (external) models.

As of this writing, five *Themes* are considered in the *Xplicit-Framework* and have been used as building-blocks of *Xplicit-Models* (Figure 17): 'Weather', 'Farmer', 'Exposure', 'EFate' and 'Effect'. Each *Theme* calculates corresponding spatiotemporally explicit outcome. Although these five themes already provide a functional basis for a range of landscape-scale risk characterisations, further *Themes* can be added to the framework later on. In current *Xplicit-Models*, the five *Themes* basically build a linear sequence in which a precursor *Theme* is regarded as independent from its succeeding *Themes* (*e.g.*, the weather is independent from all other *Themes*, eFate is assumed independent from the presence of biota and their effects). *Themes* can depend on more than one direct precursor (*e.g.*, 'eFate' can depend on exposure and weather). However, the *Xplicit-Framework* architecture allows to build more complex relationships between *Themes*.

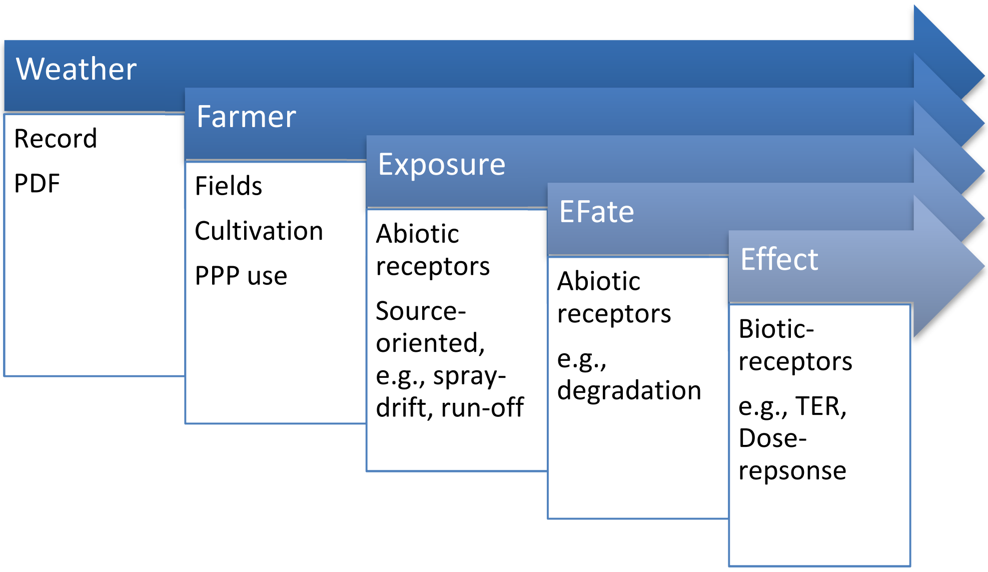


Figure 17: *Themes* and their processing sequence (with example properties or activities).

Modules representing the *Themes* operate spatiotemporally explicit (processed by *XPs*). Spatial explicitness is represented by *Receptors* as the smallest unit of analysis (Section 5.3.4.9). Temporal explicitness is represented by discrete time-steps. Modules operate by time-step, *e.g.,* at time-step t_n, a module takes its own status of time-step t_{n-1} and the status of t_n, generated by a precursor module as input (together with further data sources in case) to calculate its status for the present time-step, t_n.

5.3.3.4 Entities

Real-world objects (entities), which are relevant to the risk characterisation (directly or indirectly), are represented within the *Xplicit-Framework* as model objects (*e.g.*, farmers, fields, PPPs, habitat segments of Non-Target-Organisms (*Receptors*), etc.). This 'Object-Oriented-Approach' reflects the behaviour of the modelled system and facilitates modularity as well as stepwise introduction of context and complexity. With increasing complexity of the system, local autonomously acting entities (*e.g.*, *Receptors*) potential allow to observe emergent system behaviour at higher hierarchical levels (Grimm & Railsbeck 2005). Furthermore, properties and behaviour of natural objects can directly be transferred to model entities.

The *Farmer* entity represents cultivation practices. PPP use on *Fields* represents the primary source of potential exposure of Non-Target-Organisms. *Farmer* properties and behaviour includes, *e.g.*, field ownership, crop cultivation and PPP use. *Farmer* activities directly affect *e.g.*, exposure of *Receptors* which reside on fields.

The *Field* represents the target unit of PPP use (and further cultivation practices); hence, the *Field* is regarded as the primary target of PPP exposure. *Fields* are discretised into segments which build the smallest unit of exposure calculation (*In-field-Receptors*, Section 5.3.4.9).

Receptors are the key entity of exposure, eFate and effect calculation. *Receptors* are generic representatives of abiotic field and habitat segments, as well as of biotic Assessment Endpoints (characterising effects to Non-Target-Organisms, Section 5.3.4.9). *Receptors* represent the mathematical discretisation of the continuous spatial dimension, and hence, represent the smallest unit of numerical analysis. Abiotic *Receptors* have static spatial locations. Biotic *Receptors* can be dynamically assigned to abiotic *Receptors* during simulation runtime and, thus, can show static and dynamic spatial distributions as well. Within process models, *Receptors* are connected to (external) models that describe their behaviour. Detailed specification of *Receptor* properties and behaviour depends on the RA problem formulation and leads to a specific *Xplicit-Model* (Section 5.4).

5.3.3.5 Models

Entities' behaviour is represented by process models. Basically, process models are external mathematical models which are associated with the *Xplicit-Framework* (*Themes*) using adaptors. The association of models is an integral step of deriving a ready-to-use *Xplicit-Model* from the *Xplicit-Framework* ('customisation'). The employment of (external) process models for use in an *Xplicit-Model* depends on the RA problem formulation. Models can represent simple rules (*e.g.*, "*Farmers apply a specific PPP to land use 'wheat' between 1st and 15th April*") or sophisticated mathematical processes (*e.g.*, exposure due to spray-drift or run-off, active substance dissipation and distribution in *Receptor* compartments).

5.3.3.6 Data Services

Data access modules (services) provide external data (*e.g.*, stored in relational databases or files) to *Xplicit-Framework*-internal modules, hence, transferring external data representations into internal ones. They are also used for storing the internal state representations in external sources (*e.g.*, for exchange between modules operated by different *XPs*). Geodata provision is done by an external *Landscape-Metric* service which is of particular meaning to a landscape-scale model approach. The *Landscape-Metric* service is designed to provide the relationships between the spatial entities as necessary inputs to process models (Section 5.3.5.2).

The *Layering* pattern (Section 5.2.4.4) which requires strict separation of business logic from data endpoints is relaxed when logical functionality of data providers is utilised for efficiency reasons (*e.g.*, *XA* using SQL).

5.3.3.7 Core Library

The core library concerns the core functionality that establishes the *Xplicit-Framework* (Section 5.3.3.1). Building blocks of the core library are modular and consistently used by the *Xplicit-Components* (Section 5.3.3.2). Prominent core modules concern the management of simulation entities (*e.g.*, *Simulation-Management*, *Farmer-Management*, *Receptor-Management*), the *Task-Management* which administers the distributed computing, scale characteristics, and the provision of PDFs together with Monte Carlo sampling.

5.3.4 System Design

System design takes a more local view on the elements of the *Xplicit-Framework* and their implementation. During the iterations of the 'Agile' development process (Section 5.2.2.3), system design elements were discussed and documented up to levels that provided the basis for implementation (coding, Section 5.2.6).

In this section, major system design elements are summarised with the aim to provide a general understanding of the *Xplicit-Framework* system, which currently comprises about 300 classes.

5.3.4.1 General Design Principles

As a result of the requirement analysis (Section 5.3.2), the following primary principles guided the system design (together with the 'Pattern' in Section 5.2.4.4): Modularity and object-orientation, service-orientation, extensibility, consistency in design across modules and classes, simplicity, scalability, and adaptability.

As a key behavioural design principle, it was defined that variability within an Xplicit simulation is to be 'resolved' (*e.g.*, a value is sampled from a PDF) only at the point in space and time where necessary (taking scale-dependencies into account) and not in advance. Thus, the initialisation phase of a module does not resolve any variability that is beyond the initialization state of the simulation. For instance, the variability within the PPM calendar (Section 5.3.4.11) is resolved in the course of the simulation according to real-world farmer behaviour and not at the start of the simulation. This allows the individual simulation entity to act on current simulation conditions, hence, allow the status of an entity at t_{n+1} to depend on t_n (*e.g.*, allows a farmer to decide about PPP use on current weather conditions).

5.3.4.2 Framework Core and Xplicit-Models

The *Xplicit-Framework* core provides the key functionality of the requested spatiotemporally explicit and probabilistic risk characterisation (*e.g.*, exposure and effect calculation) that takes scale dependencies into account. Being conceptually build as a framework (Section 5.3.3.1), it has a default behaviour that results from the development requirements (Section 5.3.2). It is designed to control program flow, to call (external) models and to be extensible. An executable *Xplicit-Model* (Section 5.4) requires to associate the *Xplicit-Framework* with (external) models and services using adaptors and a configuration.

Providing the key functionality, the *Xplicit-Framework* core is employed in the *Xplicit-Management* (*XM*), the *Xplicit-Processor* (*XP*), and the *Xplicit-Assess* (*XA*)) *Components*.

Key modules of the *Xplicit-Framework* core are shown in Figure 18. From an operational viewpoint, the three colours in Figure 18 represent a *3-Operator-Roles* concept that defines and separates the roles of (i) the *Xplicit-Framework* developer (including, *e.g.*, business requirements, software architecture, system design and implementation), (ii) the role of the *Xplicit-Model* developer (including, *e.g.*, model definition, adaptor development and configuration), and (iii) the *Xplicit-Model* user (*e.g.*, trained modeller or risk assessor). The latter uses an *Xplicit-Model* (Figure 19) by parameterisation via an *Xplicit-Frontend* (*e.g.*, editor, web browser).

Figure 18: Schematic *Xplicit-Framework* modules and their association to the *3-Operator-Roles* concept (dark brown = *Xplicit-Framework* module, light brown = associated model or module, green = modules and services defined by the user of an *Xplicit*-Model, 'Config.' = configuration, with aspects of the framework and associated models).

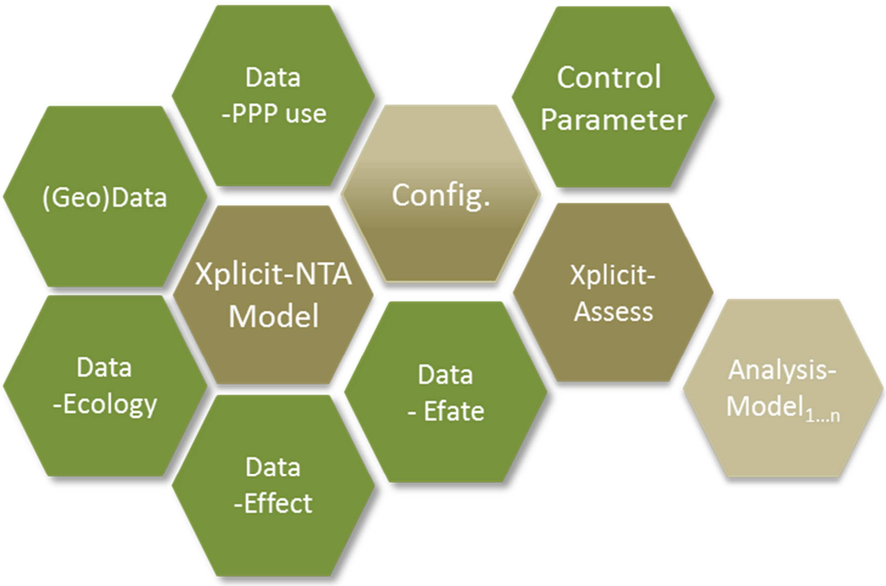


Figure 19: Schematic example *Xplicit-Model* modules and their association to the *3-Operator-Roles* concept (dark brown = *Xplicit-Framework/-Model* module, light brown = associated model, green = modules or services defined by the *Xplicit-Model* user, 'Config.' = configuration, with aspects of the framework and associated models).

5.3.4.3 Xplicit-Management and Xplicit-Processors

Xplicit-Components are introduced in the architecture section (0). *Xplicit-Management* (*XM*) and *Xplicit-Processors* (*XPs*) basically share the same *Xplicit-Framework* core code and build the actual Xplicit simulation unit (*Xplicit-Engine*).

XM builds the central unit of an Xplicit simulation. *XM* initialises an Xplicit simulation and prepares its processing within the distributed computing environment (*e.g.,* prepare and deploy processing tasks for *XPs*, collect and combine the results of *XPs*). From a design perspective, *XM* was developed as a kind of middleware (Schäfer 2010), an intermediary unit between the independent *XPs*: Processing of *Themes* (designed as modules, *e.g., Farmer, Exposure, Efate, Effect*) resembles a Pipe-and-Filter pattern (Schäfer 2010) having *XM* compiling the time-step results of the *XPs* which serve as input for subsequent *Themes* (and time-steps). *XM* itself is represented by a module (implemented as class `XMProcessorModule`), which inherits from the abstract class `ProcessorModule`. *XM* is currently operated as the sole compiling instance of *XPs*' output. However, modularisation has been implemented in a way that allows *XM* to configure *XPs* as compiling instances that focus on specific *Themes*, in order to further improve options for parallel processing, hence, to improve performance and scalability.

XPs represent the actual simulation units. *XPs* are designed to independently conduct defined spatiotemporally explicit calculations that are restricted to a specific *Theme* and a defined part of the entire landscape. *XPs* are designed to listen to a task channel, to pick tasks from that channel (Section 5.3.4.14), to initialise the modules necessary for performing the task, to load the necessary data, to actually conduct the calculations, to write the output for each individual time-step to a central project repository and to autonomously reset their status after task completion (and to start listening to the task channel again).

XPs have the capability to process any configured *Theme* of an Xplicit simulation (*e.g., Farmer, Exposure, Efate, Effect*, defined in a class `ThematicModuleConfiguration`), *i.e.*, an *XP* is omnipotent regarding the themes it can process. However, individual *XPs* can also be restricted to one or more specific *Themes*. An *XP* is represented by a module, and implemented as class `XEProcessorModule`, which inherits from the abstract class `ProcessorModule.` The *Theme* which an *XP* is processing is determined by the task it picks from the task channel.

Object exchange between runtime instances makes use of serialisation and deserialization (CodeProject 2012, Microsoft 2012d).

5.3.4.4 Xplicit-Assess

Xplicit-Assess (*XA*) is the *Component* to analyse the outcome of an Xplicit simulation with the aim to provide the requested risk characterisation. The *XA* module is designed to operate as a stand-alone process that can be part of an Xplicit project. *XA* is capable to aggregate *XE* outcome in different risk dimensions (*e.g.*, maximum PEC(receptor) over simulation time), to combine simulation results with further landscape data (*e.g.*, building *Receptor* groups at different scales), to store results in central databases and to conduct statistical analysis (*e.g.*, distribution of probabilities of a defined endpoint to exceed a trigger value) (example evaluations are provided by the case studies, Section 6).

XA is implemented as class `XAProcessorModule` which inherits from the abstract class `ProcessorModule.` *XA* itself is of modular design where each module represents a single assessment step. Modules can be added for further analysis. *XA* processing is defined and operated as an 'assessment tree'. The root of the tree is given by the initial data source for the assessment whereas each node of the tree represents a single assessment command. The outcome of each node is passed to the next node along the tree branches. Branching the tree enables to pass the result of a command to multiple subsequent commands. *XA* further on allows to process multiple assessment trees within one instance (*i.e.*, they are processed independently and in sequence).

XA is configured by XML. The *XA* module configuration consists of one child element `Assessments`, which is the list of assessments that are sequentially conducted by the `Assessment` processor. Each assessment is configured by two child elements, `DataSource` (data location; any *XA* `DataSource`) and `Commands` (commands that are applied to the data). A `Command` can include, *e.g.*, internal code, external models, SQL statements, R-scripts (CRAN 2011), geoprocessing. The design allows to introduce further commands and implement analysis steps as services (*e.g.*, Section 5.3.5.6).

5.3.4.5 Simulation-Management and Configuration

The *Simulation-Management* represents the status of an Xplicit simulation. The class `SimulationManagement` holds the 'simulation environment', *i.e.*, instances of different modules (*e.g.*, weather, data access and service managements), as well as the current simulation status (*e.g.*, simulation time management). The *Simulation-Management* can reset itself.

The project configuration (classes `ProcessorConfiguration`, `ProjectConfiguration`) is initialised via de-serialisation of an XML configuration. The XML configuration defines the *Xplicit-Model* (Section 5.4) with its modules, including, *e.g.*, the *Themes* considered by *Xplicit-Processors*, specification of the control channels used for distributed computing, and general simulation parameters. The configuration can be split into multiple parts and can partly be represented in different ways (currently as XML and plain text). The modularity of the configuration allows to specify those parts that are accessible and changeable by the user via *XF*. The XML of the configuration is described by an XSD (XML Schema Definition) which is also used to check the validity of a configuration.

A configuration can also include invocation of an *XA* configuration in order to run an entire Xplicit simulation project from a single *XF* call (*e.g.*, by a web-server after initiation from a client web page).

5.3.4.6 Main

The *Main* method of a processor module is called after initializing an instance of the `SimulationManagement` class and performs all higher-level actions of the module. It requires a reference to the `SimulationManagement` object and thus has access to the simulation environment.

In an *XP*, the core of the *Main* method is an endless loop. As a result, an *XP* does not terminate until forced by the user or by a specific 'shut-down' *Task* provided by *XM* (or due to a fatal exception). A single loop performs a single *Task* (Section 5.3.4.14) after which the `SimulationManagement` object is reset.

5.3.4.7 Modules

Modules encapsulate properties and behaviour of major units of the *Xplicit-Framework* and occur at different system levels: *e.g.*, simulation *Themes* (*e.g.*, weather, farmer, exposure, eFate, effect, Section 5.3.3.3), services (*e.g.*, *Landscape-Metric*, Section 5.3.5.2), assessment commands (Section 5.3.4.4) or *Receptors*. Modules are derived from the abstract base class `XplicitModule`.

5.3.4.8 Managements

The necessity to manage the inherent complexity of a landscape-scale model approach has become apparent in early iterations of the agile development process (Section 5.2.2.3). On this background, a management level was established in different modules.

Responsibility of the management with respect to its managed entities include, *e.g.*, configuration, initialisation, passing status information to the managed entities (*e.g.*, current time-step), specific activity requests to entities (*e.g.*, status reporting) and mediation between entities behaviour. Managements of higher-level modules are referenced by the *Simulation-Management* (Section 5.3.4.5).

Example *Management* classes: `SimulationManagement`, `ReceptorManagement`, `TaskManagement`, `WeatherServiceManagement`, `FarmerManagement`, `ExposureManagement`, `EffectManagement`, `DataAccessManagement`, `PpmManagement`.

A *Management* can be regarded as an *Xplicit-Framework* internal service, and hence, provides a technical prerequisite to transfer modules into service endpoints in the future.

5.3.4.9 Receptors

Receptors are key entities of the Xplicit approach. Abiotic *Receptors* result from the discretisation of the landscape, and hence, represent segments of real-world land use/cover. *Receptors* are initialised in *Xplicit-Models* via a *Landscape-Metric* service (Section 5.3.5.2). Numerically, *Receptors* represent the smallest spatial unit of analysis.

Abiotic *Receptors* are represented by entity objects of type `ReceptorAbiotic`, yet, the specific properties of each receptor type are defined in the model configuration using a module of class `ReceptorAbioticDefinition`. Specific abiotic *Receptor* classes are derived from this abstract class (*e.g.,* habitat segments of Non-Target-Arthropods were defined in class `ReceptorAbioticTerrestricSimple1Definition` in the example study in Section 6.1, or class `ReceptorAbioticAquaticSimple1Definition` which was designed to represent simple water body segments in example study Section 6.4).

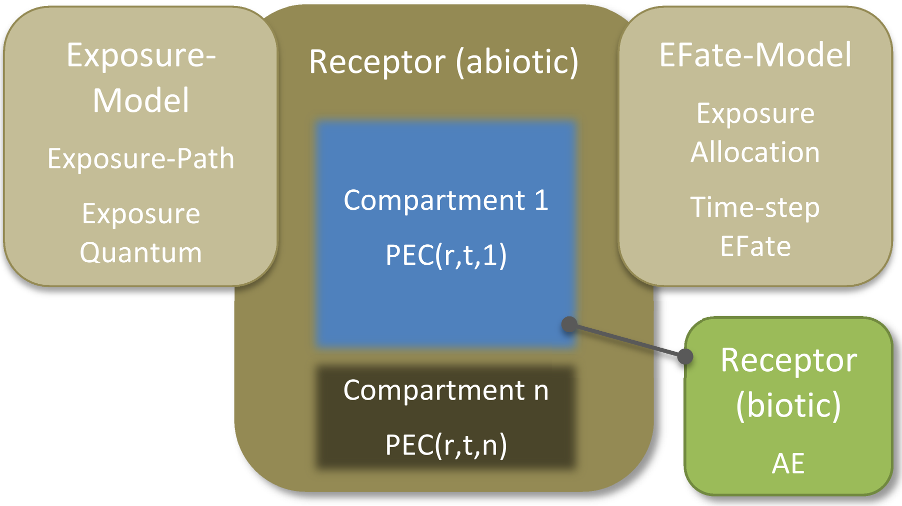


Figure 20: Illustration of an abiotic *Receptor* in relation with exposure and eFate models, as well as a biotic *Receptor*. (PEC(r,t,1) = Predicted Environmental Concentration of *Receptor r*, at time *t*, in *Compartment 1*, AE = Assessment Endpoint).

The interaction of abiotic *Receptors* with other modules is illustrated in Figure 20. Abiotic *Receptors* are related to *Exposure-Paths* (Section 5.3.5.3) by which they receive exposure quantums (class `ExposureQuantum`, defining an active substance, its amount together with a unit). Exposure paths are entities initialized in the context of exposure models (Section

5.3.4.10) to represent the spatial behaviour of exposure. After being affected by an exposure quantum, a *Receptor* distributes the exposure to its *Compartments* (*e.g.,* to calculate initial concentrations for a *Compartment*). *Compartments* are, thus, the properties of a *Receptor* that receive and store concentrations. The translation of exposure quantums to concentrations is part of an initial eFate process which is represented by a process model ('allocation model'). The initial eFate process needs to be capable of calculating initial concentrations, which are conceptually assumed to occur instantaneously and are required in regulatory risk characterisation (following assumptions to assure conservatism, Section 4.3), and to calculate environmental fate of active substance in time-steps. *Receptor* instances are managed by a *Receptor-Management* (Section 5.3.4.8). Further major design aspects of abiotic *Receptors*:

- Abiotic *Receptors* have a static location (represented by a number (ID)), either without, or with model-world or real-world coordinates.
- Abiotic *Receptors* are in topological relationship to further model entities (*e.g.*, *Exposure-Paths*, Section 5.3.5.2).
- Abiotic *Receptors* contain *Compartments* (class `Compartment`) which represent relevant real-world properties and behaviour, and which store and report PECs(t) (t = time). Abiotic *Receptors* can act as a sink and source of exposure.
- *In-field-Receptors* and *Off-Crop-Receptors* are prominent abiotic *Receptors* derived from the base class.
    - The agricultural field is the primary unit of exposure events. *In-field-Receptors* are field segments, hence, are initially exposed in a PPP application event. *Compartments* of *In-field-Receptors* can represent *e.g.*, 'air', 'plants' and 'soil', and are related to corresponding eFate models (*e.g.*, *Compartment* air is the source for spray-drift exposure, *Compartment* 'plants' can intercept fractions of the sprayed PPP volume and *Compartment* 'soil' is the source for run-off modelling).
    - *Off-Crop-Receptors* represent abiotic habitat segments of Non-Target-Organisms.

Biotic *Receptors* represent Assessment Endpoints (biological entity and attribute, Suter 2007) which can be any endpoint defined by protection goals and in the RA problem formulation (Section 4.3, *e.g.*, TER, dose-response relationship, population abundance). Biotic *Receptors* can be statically or dynamically assigned to a *Compartment* of an abiotic *Receptor* (class `ReceptorBioticGeographicRelationServiceDefinition`).

5.3.4.10 Associated Models

In the *Xplicit*-Framework, a 'model' can be regarded as a function that describes ('models') the behaviour of a (natural) system (basically by mathematical means and numerical processing). Models carry service characteristics and are represented in the framework by modules. Models which are part of the *Xplicit-Framework* core are technically referred to as *Internal-Models*, such which come as external code (.dll, .exe) or services are called *External-Models*. Conceptually, both are referred to as *Associated-Models*.

Prominent examples for *Associated-Models* are exposure, eFate and effect models, represented by the abstract classes `ExposureModel`, `EfateModel`, and `ReceptorBioticEffectModel` which all inherit from `XplicitModule`.

Example exposure models are the Schad & Gao model for spray-drift depositions (Section 5.3.5.4, class `ExposureSprayDriftPdfSchadGaoLumpedModel`) or run-off models (*e.g.*, 'Exposit-Type', Großmann 2008, class `ExposureRunoffExpositSimple1Model`, implemented as `ExternalExposureModels.dll`). Classes of instantiable exposure models inherit from class `ExposureModel`. Exposure models use *In-field-Receptors* as the primary source of exposure and calculate exposure along *Exposure-Paths* which are provided by a *Landscape-Metric* (Section 5.3.5.2). Yet, the behaviour of abiotic *Receptors* can be extended in such a way that different types of abiotic *Receptors* can provide a source of exposure. In an *Xplicit-Model*, multiple exposure models can be configured and used simultaneously (representing different exposure routes, *e.g.*, spray-drift and run-off).

Spray-drift filter models represent a further important model type in the calculation of exposure (Section 5.3.5.5, `Simple1DriftFilterModel`).

Substance dissipation due to adsorption and degradation is a prominent process modelled by eFate models (*e.g.*, FOCUS 2001). EFate models are referenced by abiotic *Receptors*.

Effect models describe Assessment Endpoints (Suter 2007) and are referenced by biotic *Receptors*. Simple effect models are, *e.g.*, TER (class `ReceptorBioticTerEffectModel`), RQ (Risk-Quotient, class `ReceptorBioticRQEffectModel`) and dose-response models (class `ReceptorBioticDoseResponseLogLogisticEffectModel`). Instantiatable effect model classes inherit from the abstract base class `ReceptorBioticEffectModel`.

Association of *External-Models* to the *Xplicit-Framework* generally requires the development of a specific model adaptor (Figure 21). This adaptor allows to configure and control the *External-Model* (*e.g.*, initialisation, start, time-step, termination), as well as to exchange data (model in- and output). The *External-Model* can autonomously access further data sources (*e.g.*, environmental data). However, only data that is exchanged via the *Xplicit-Framework* can be subject to *Uncertainty-Analysis/Sensitivity-Analysis* (Section 5.3.4.13).

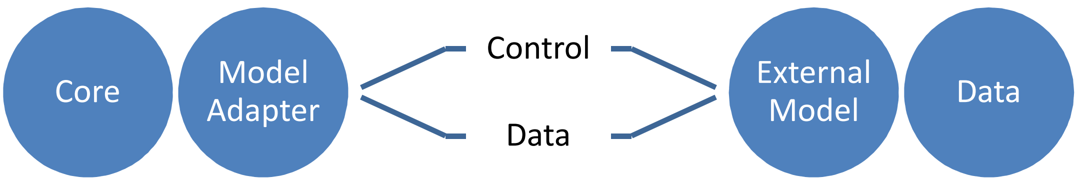


Figure 21: An *External-Model* is associated to the *Xplicit-Framework* via a model adaptor.

5.3.4.11 Farmer-Module

The *Farmer-Module* simulates cultivation related entities and their behaviour, including, *e.g.*, field management and PPP use. A farm is regarded as a unit with internal properties and an internal behaviour and is represented by a *Farmer* module. The *Farmer-Management* (Figure

18, Section 5.3.4.8) is the instance that manages *Farmer*s (*e.g.,* informs farmers on simulation time-step and ask them for certain activities).

As of this writing, the following *Farmer* properties and behaviour have been implemented:

- Farm size: Different options of field-to-farmer association (during simulation initialisation), comprising 1:1 and n:1 field-to-farmer association, with random and or deterministic association (using geodata) and taking field types into account.
- Crop-rotation: In typical temporal scales of risk characterisation (≈10^0-10^1 years, depending on regulatory requirements, Section 4.3). Crop-rotation is especially relevant to arable farming; thus, crop-rotation schemes can be configured taking land use statistics at regional scale into account (using geodata).
- Plant protection measures (PPM): The ultimate goal of Xplicit is to support risk characterisation for potential ecological effects caused by the use of PPPs. Thus, the PPP use module represents a core farmer activity. Each farmer builds its personal PPM calendar, which consists of determined and variable (probabilistic) elements (*e.g.,* PPP choice, application timing and rate, exposure reduction). Variable (probabilistic) elements are resolved (get determined) at spatiotemporal simulation 'points' (temporal and spatial), taking scale dependencies into account as they are defined in the configuration. For instance, the determination of the PPM calendar as such can be configured to occur at the start of a season whereas the decision on individual PPP applications can be configured to be determined within an application time window (resolving the corresponding PDF). Thus, the system models potential real-world farmer behaviour. PPM calendar elements and structure (Figure 22) allow to define a wide range of PPMs, including, *e.g.*, simple and complex plant protection schedules, organic farming, market share of a PPP, tank mixes, etc. The PPM calendar is implemented by individual classes which are interrelated according to the structure shown in Figure 22. At the current level of implementation, the PPM calendar allows to consider the following variability:
  - Variability of PPMs in PPM calendar: At a given point in time, the farmer has to determine his actual PPM calendar by sampling a PMF of available PPMs. This allows for variability regarding PPMs among farmers.
  - Variability of application sequences of a PPM: At a given point in time, the farmer has to determine the application sequence of a specific PPM. This allows for variability between applications in a sequence (*e.g.,* a PPP label allows for up to *n* applications).
  - Variability of the individual application: The determination of the individual application corresponds to the real-world situation when the farmer has prepared his/her sprayer and is ready to conduct the application. At this point in time, the application technology, the PPP(s) in the sprayer tank, their individual use rates and the timing become determined.

  Sample cases:

  - Simple case: 1 PPP containing 1 active substance, used in 1 crop at 1 use rate, by spraying and all farmers: PPM calendar has 1 PPM, consisting of 1 application sequence (*e.g.,* 2 applications, each within a 10 day time-window defined by an uniform PDF specifying the actual application timing).

- Complex case: The PPM calendar of individual farmer comprises different PPMs for different crops, each with application sequences for different PPPs, some of which are combined into single PPP uses (tank mixes).

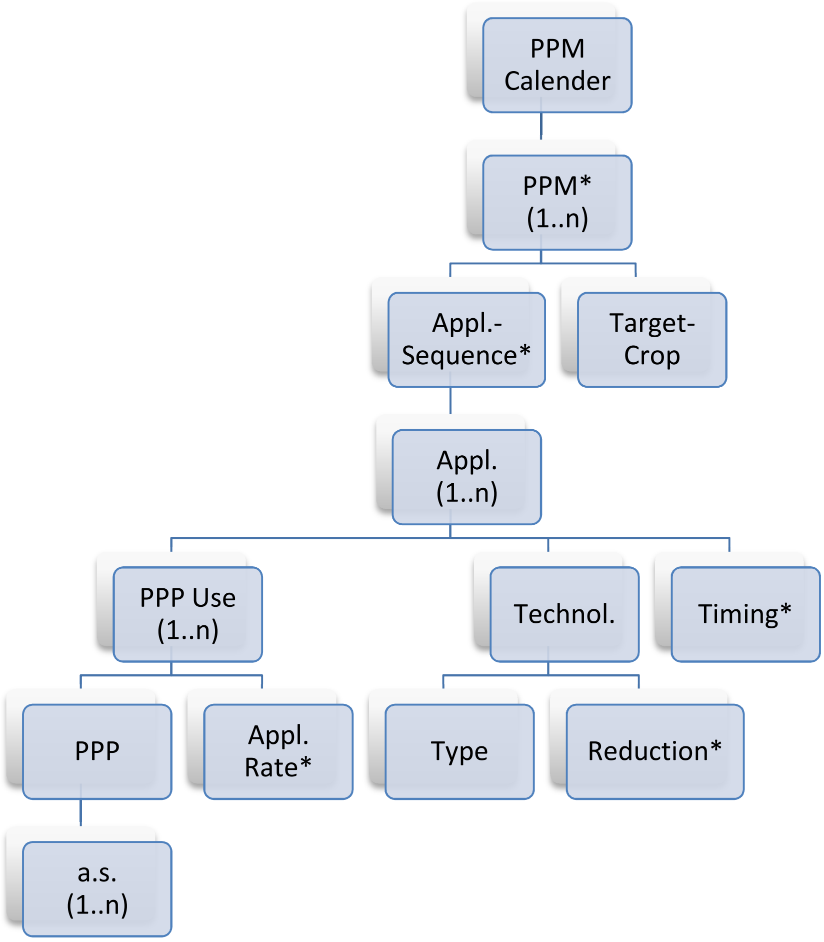


Figure 22: Structure of a PPM calender. A higher-level entity is composed of those following in the hierarchy. '(1..n)' indicates that multiple entities of this type can occur. Further abbreviations: 'PPM' = Plant Protection Measure, 'Appl.' = application, 'Technol.' = application technology, 'Type' = application type (*e.g.,* spray, soil incorporation, granule, etc.), 'Reduction' = exposure reduction factor, 'a.s.' = active substance, '*' = definition includes variability (PDF, PMF, *Spatiotemporal-Signature*, Section 5.3.4.12).

The *Farmer* module is designed to be extended by further farmer properties and behaviour, *e.g.*, field management (harvesting, ploughing) or RM practices (*e.g.*, maintenance of riparian vegetation as a filter for spray-drift) which can be considered relevant to ecological risk characterisations and allow a further improvement of the assessment of co-occurrence of exposure and sensitive life stages in space and time (Section 4.3.1).

5.3.4.12 Variability

The term variability represents natural variation of a state variable of a given system and observation scale (*e.g.*, wind direction at field scale during application, spray-drift deposition at field scale, application timing at PPM scale), whilst uncertainty represents our incomplete knowledge about the true value of that state variable. Only the latter can be improved by more accurate measurements or observations. Variability of environmental and agricultural conditions is considered to cause large spatiotemporal variability of species risk (Verdonck 2003, Section 4.5). Consequently, the propagation of that variability to risk characterisation is a key goal of the Xplicit development.

The concept of probability is used to characterise risk (Morgan & Henrion 2007, Section 4.3.1 and 4.5.5). Probability is estimated using a frequentist approach, *i.e.*, the probability of an event to occur is estimated from the frequency by which it occurs in a sequence of trials. The sequence of trials is realised using a Monte Carlo approach (Morgan & Henrion 2007).

Variability is represented in distributions (Probability Density Functions (PDFs), or Probability Mass Functions (PMFs), abstract class `PDF`, Figure 23). Class PDF supports the usage of a seed and the choice of a random number generator (*e.g.*, High quality random number Mersenne-Twister, XOR shift, CodePlex 2012). Actual PDF distributions are represented by classes and are derived from a base class for discrete or a base class for a continuous PDF, respectively (Figure 23). Distribution classes were adopted using the code of the MathNet.Numerics project (CodePlex 2012, "*Numerics is the numerical foundation of the Math.NET project, aiming to provide methods and algorithms for numerical computations in science, engineering and every day use.*").

Variability can basically be assigned to any *Xplicit-Model* parameter using the configuration XML (*e.g.*, wind direction, PPP application rate, yet, also decision parameters like PPM decision, Section 5.3.4.11).

A key characteristic of variability (and uncertainty) is its scale dependency (Section 4.4 and 4.5), *e.g.*, empirical variability of spray-drift deposition might differ (and can therefore be described) at local, field, or field-ensemble scale (Section 5.3.5.3). Therefore, a *Spatiotemporal-Signature* was developed which represents the spatiotemporal scales represented by a PDF and, thus, the spatiotemporal scales for which samples can be drawn from it. Values to which variability is assigned to are held in the class `PdfQuantity`, deterministic values are held in the class `DeterministicQuantity`. Both classes inherit from the abstract class `Quantity` which provides the properties `Unit` and `SpatiotemporalSignature`. Class `SpatiotemporalSignature` represents a spatial and a temporal signature (scale) that is composed of members from the enumerations `SpatialScalesInProject` (*e.g.,* 'StudyRegion', 'Field', 'Receptor', 'Farmstead') and `TemporalScalesInProject` (*e.g.,* 'TenYears', 'Year', 'Month', 'Week', 'Day', 'Hour', 'Season').

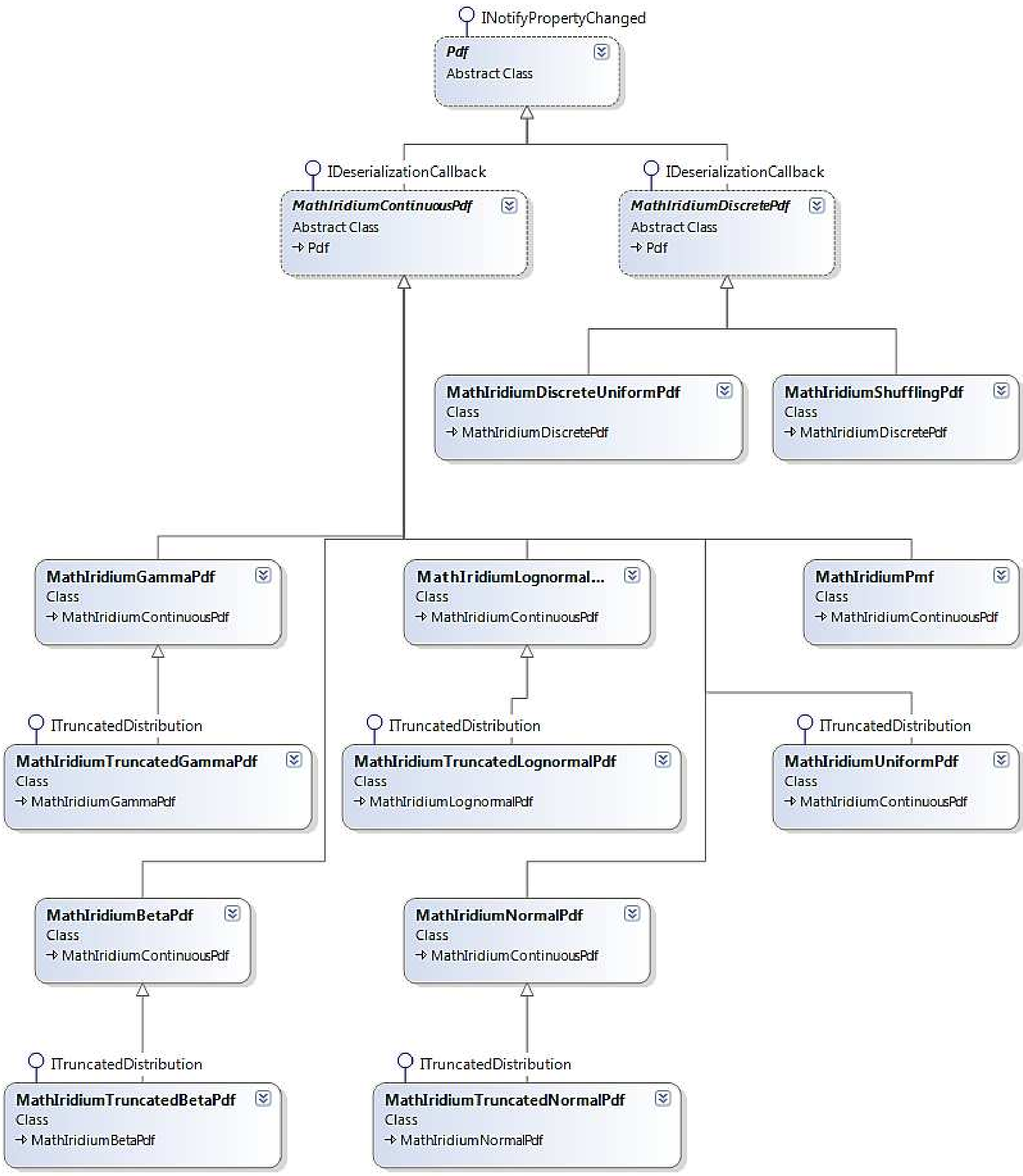


Figure 23: PDF class diagram.

When a sample is requested from an instance of a `PdfQuantity`, the requesting object announces its spatiotemporal identity (*i.e.*, a collection of spatiotemporal units it is member of) and the `PdfQuantity` instance checks whether its own spatiotemporal signature fits the spatiotemporal identity of the requesting object. If so, a value from the PDF is considered to validly represent the state of the requesting object. In this case, the `PDFQuantity` checks whether a value for the requested spatiotemporal scale was previously requested and returns the earlier drawn cached value or, if the request for a value is the first for a spatiotemporal unit, it draws and provides a new sample. For example, a PDF representing spray-drift variability across *Exposure-Paths* scale (Section 5.3.5.2) will return new samples only at *Exposure-Path* scale but not below, on *Receptor* scale as member of the same *Exposure-Path*. Given a PMF representing variability of discrete wind directions at regional scale across fields, different wind directions are sampled for different fields, but not for, *e.g.*, different *Exposure-Paths* of the same field. Likewise, a PMF representing temporal variability of discrete cropping decisions of farmers that have a temporal signature of 'year', will return the same value for every time-step within a year, but different samples between years. The spatiotemporal scales represented by a PDF can be defined by the user in the XML configuration.

5.3.4.13 Uncertainty-Analysis/Sensitivity-Analysis

Parameter uncertainty refers to uncertainty of the true value(s) of model parameters (Section 5.3.4.12, Warren-Hicks & Hart 2010). Propagation of parameter uncertainty (uncertainty analysis, UA) aims at exploring the range of model outcome (and the probability of occurrence) whereas sensitivity analysis (SA) aims at assessing and quantifying the impact of parameter changes. Technically, both analyses can be addressed using the same *Uncertainty-Analysis/Sensitivity-Analysis* (UASA) approaches.

A 2nd-order Monte Carlo approach has been implemented to conduct UASA in the *Xplicit-Framework* and so, to distinguish between variability and uncertainty (Section 5.3.4.12). A 2nd-order Monte Carlo approach consists of two loops, an inner loop which represents variability and an outer loop which represents parameter uncertainty. The inner loop of variability propagation is described in Section 5.3.4.12. The outer UASA loop covers uncertainty that is not resolved during actual Xplicit simulation (Monte Carlo) runs but that is resolved prior to the distribution of working tasks (Section 5.3.4.14). The initial project configuration, thus, contains two distinct kinds of uncertainty, whilst the working tasks received by *XPs* only show Monte Carlo run variability (inner loop). Implementation of UASA, thus, required to enable *XM* to resolve uncertainty prior to working task deployment. Basically, any parameter can be configured as subject to UASA using the distributions introduced in Section 5.3.4.12 (class `ConfigurationValue`). *Xplicit-Assess* (*XA*, Section 5.3.4.4) is capable to evaluate UASA in correspondingly configured assessment trees. Furthermore, entire modules in the XML configuration can be subject to UASA (classes `ConfigurationModule<T>`, `ConfigurationList<T>`) which can be of particular interest to *Sensitivity-Analysis.*

5.3.4.14 Distributed Computing

Scalability is among the major non-functional requirements (Section 5.3.2). Landscape-scale risk characterisation is ideal for parallelisation as it performs a large number of similar calculations across landscapes (*e.g.*, spray-drift exposure from sprayed fields). Concepts for *Distributed-Computing* for 'on-premises' distribution of parallel tasks, developed in early iterations of the Agile development cycle (Section 5.2.2.3), were found to be largely in line with already existing queue-based systems (*e.g.*, Microsoft Azure (Microsoft 2013), Jennings 2009, Krishnan 2010, Sirtl 2010, Hay & Prince 2011). These concepts were adapted in view of operating *Xplicit-Models* at the Microsoft Windows Azure platform.

Design aspects of the *Distributed-Computing* functionality (*Xplicit-Framework* core, Figure 18):

- *Xplicit-Project*: An individual Xplicit simulation, using a specific *Xplicit-Model* and -*Scenario* (Section 5.4), defines an *Xplicit-Project* which has a unique ID assigned (GUID, Globally Unique Identifier). All project related processing steps are identified by this GUID (*e.g.*, processing, evaluation, administration).
- *Roles*: *XPs* have the role of processors (Section 5.3.4.3, 'worker role' in Microsoft Azure), *i.e.*, *XPs* conduct the actual model calculations. Typically, a number of *XPs* process an Xplicit project in parallel. *XPs* can be added during *Xplicit-Project* runtime. After *Task* (below) completion, an *XP* is reset. *XM* has a management role. *XM* initialises an *Xplicit-Project*, prepares and deploys *Tasks*, compiles results of *XPs*, and terminates a project. Typically, a single instance of *XM* manages a single *Xplicit-Project*. *XM* is also designed to redirect data compilation *Tasks* to *XPs*.
- *Message* channel: *Tasks* and *Messages* (below) are prepared and put into a channel (by *XM*). The concept is independent from its implementation. 'On-premises', *i.e.*, in an intranet of servers (or Personal Computers, PCs) which can access a central file drive, the channel is implemented to operate with files as *Messages* and *Tasks*, whereas at Windows Azure the corresponding services are used (Microsoft 2013).
- *Tasks*: A *Task* is built by an *Xplicit-Model* configuration for a certain *Theme* (Section 5.3.3.3) and the definition of a subset of the spatial study domain (typically a set of fields or *Receptors*; no partitioning over the temporal domain). *Tasks* are prepared by *XM*, typically as a result of splitting the entire landscape to be processed and are processed individually by single *XPs*. A *Task* is identified by a GUID. The workload of *Tasks* (*e.g.*, number of entities to be processed) can be adapted to machine resources.
- *Messages:* Small text messages are posted by entities of a *Distributed-Computing* environment in certain communication channels (*e.g.*, a *Task-Message* is posted by *XM*, informing *XPs* about a new *Task* that has been published). A *Task-Message* contains metadata, *e.g.*, to characterise the *Task* processing priority. A *Task-TimeStepFinalised-Message* is posted by *XM* to inform *XPs* that processing of time-step t_i has been done for a certain *Theme* (by UASA run number, Monte Carlo run number). *XM* can post *XP-ShutDown-Messages* to *XPs*, which will cause them to terminate their execution. Basically, *Messages* are deleted by the entity that has picked the *Message*.
- *Shared-Counter*: The *Shared-Counter* provides a means to keep track of *Xplicit-Project* processing and is implemented as a central table, accessible by *XM* (read-access) and *XPs* (write-access). The Shared-Counter may reside at any data location supported by the *Xplicit*-Framework, *e.g.*, central database. *XPs* report their *Task* completion to the *Shared-Counter*. *XM* observes the *Shared-Counter* in order to react on the completion of *Tasks* for individual time-steps (by UASA run#, Monte Carlo run#, *Theme*).
- *Task* processing rules: Typically, a large number of *Tasks* are generated in course of an *Xplicit-Project* and are posted to a *Message* channel. Picking *Tasks* by *XPs* follows simple rules which assure that *Xplicit-Projects* get effectively processed. For example, "pick a *Task* from the lowest available UASA run#, in this, from the lowest available Monte Carlo run#, in this, from the *Theme* of highest priority (example priority sequence

'weather', 'farmer', 'exposure', 'effect'); in case prioritisation rules result in >1 possible *Tasks* (due to parallelisation of spatially splitting the landscape) then choose one of these randomly."

- Timeouts: *XM* monitors the processing time of individual *Tasks*. In case the processing time of a *Task* exceeds a configured threshold, the *Task* is published again by *XM*. System idempotency assures that the system keeps its state in case a *Task* is processed more than once. Timeout is also assigned to the entire *Xplicit-Project*. In case of *Xplicit-Project* timeout, *XM* shuts-down project execution.
- Data storage: Outcome of *XPs* can be stored at any data location supported by the *Xplicit*-Framework. Binary files are used 'on-premises' with a central storage for performance reasons ('Blobs' at Microsoft Azure).

Robustness (as a non-functional requirement, Section 5.3.2) of the *Distributed*-Computing design has been proven in different *Xplicit-Projects* (*e.g.*, Section 6). The *Distributed-Computing* environment is represented by the following major classes: `DataAccessManagement`, `TaskManagement, Task, Message, Project, Theme, Uasa, MCrun`.

5.3.4.15 Data-Access

A data layer module (data service) was established in order to keep data processing in the business-logic layer (actual mathematical modelling) of the *Xplicit-Framework* separate from external data schemes and their physical sources (Section 5.2.4.4). The data layer is mainly represented by class `Xplcit.IO`.

As of this writing, binary files, text files, XML files, database (RDBMS, Oracle (Oracle 2012), Microsoft SQL Server (Microsoft 2012a)) and Microsoft Azure storages (Microsoft 2013) have been used as physical data sources.

5.3.5 Associated Models and Services

Associated-Models represent models and services which provide a defined functionality (*e.g.*, mathematical modelling of a natural system, geo-processing, Section 5.3.4.2 and 5.3.4.10). The term '*Associated*' indicates the concept that these models can be associated to the *Xplicit-Framework* core. Prominent examples for *Associated-Models* are *Receptor*, farmer, exposure, eFate or effect models. *Associated-Models* are necessary to derive ready-to-use *Xplicit-Models* from the *Xplicit-Framework*.

This section introduces example *Associated-Models* which have been developed in the course of the *Xplicit-Framework* development and which have been employed in *Xplicit-Models* (Part 3, Section 6).

5.3.5.1 Overview on *Associated-Models and -Services*

The development of *Associated-Models* so far has been focused on models and services which were essential to establish a basic landscape-scale model approach as requested (Section 4.5

and 5.3.2) and to define *Xplicit-Models* addressing current RA problems with a focus on a stepwise introduction of landscape-scale context (*AutContext*, Section 4.2).

Table A 3 (Appendix 11.2) provides an overview on *Associated-Models* and *-Services* which have been implemented and employed (Part 3, Section 6) so far.

5.3.5.2 *Landscape-Metric* Service

Spatially explicit landscape-scale exposure and effect modelling depends on adequate geodata with respect to, *e.g.,* thematic representation of relevant entities, spatial resolution and up-to-dateness. The spatial relationships of discretised entities are of particular importance to local landscape-scale exposure and effect modelling. Therefore, actual modelling of processes can be regarded as a client of a geodata preparation service. This perspective leads to the basic idea of a *Landscape-Metric* service. Modelling and service modules can be located in separate institutions which can positively affect geodata licensing and can facilitate harmonisation of landscape-scale risk characterisation approaches (Section 4).

In summary, a *Landscape-Metric* service has been developed with the following characteristics:

- Objective: Development of concepts for a *Landscape-Metric* service for landscape-scale risk characterisation modelling and implementation for spray-drift and run-off exposure modelling, as well as for scale-dependent evaluation of *Xplicit-Model* outcome (*XA*, Section 5.3.4.4).
- The *Landscape-Metric* is part of the Xplicit modelling approach. As of this writing, version 3 has been implemented ('LM3').
- The *Landscape-Metric* service is an integral building block in a modular geodata preparation sequence. It provides spatial data as *Xplicit-Model* input: base geodata, processed geodata, data topology.
- The architecture of the service (Figure 24) follows the SOA approach (Section 5.2.4.5).
- The *Landscape-Metric* service was implemented as an *ad hoc* service, *i.e.*, its outcome is generated and provided on demand and is stored only temporarily (cached).
- The actual *Landscape-Metric* content provides a topology that represents the spatial relationships entities as required by model processes (*e.g.*, local crop-to-water body distance, local crop-to-terrestric habitat distance). The metric is defined by a conceptual contract and represented by according classes. From an operational point it can be viewed as a service, from a conceptual viewpoint as a semantic model.
- The *Landscape-Metric* service is extendable to further model input requirements, *e.g.*, to characterise and process biotic receptors.

Objectives and Requirements

Major aspects of the requirements analysis of the 'LM3' version of the *Landscape-Metric* service are summarised in Table 7. The development process followed an Agile development process (Section 5.2.2 and 5.2.3).

Table 7: Aspects of the 'LM3' requirements analysis.

Topic	Aspect
Business	Geodata service to provide geodata (topology) as immediate input to Xplicit landscape-scale risk characterisation modelling. Cost reduction due to standardisation and automation of processes. Foundation for future harmonisation and institutional separation of base geodata owners and processed geodata clients (improved licensing). Good system maintenance.
Concept	'*Mapping of base geodata into landscape-scale model input*'. Separation of (i) base geodata (*e.g.*, land use/cover), (ii) processed geodata (*e.g.*, habitat types), and (iii) data topology as direct model input (*e.g.*, discretised, non-georeferenced local crop-to-habitat segment distances).
Operation	Principle: '*Base data in – topological data out*'. Initially, GIS processing steps as well as LM3 generation and compilation as manual operation sequence. Automation with stepwise integration into a single server-based process. Operation steps include splitting of large study regions into portions (operation in parallel computing), discretisation of geodata entities, *Exposure-Path* generation (below), analysis of spatial relationships, development of topology and temporal storage (*ad hoc* service). Module operations can be distributed across a network. Output is provided by a central storage or http-endpoint (*e.g.,* Oracle 2012, Microsoft 2013, file drive) and is accessed by Xplicit (*XE, XA*, Section 5.3.4).
Semantic geodata	Data provided by the service should consist of spatial relationships between landscape objects (topology) as defined by their relevance to exposure and effect modelling and as resulting from the numerical discretisation of the continuous real-world entities (*Receptors*, Section 5.3.4.9). The attributes provided by the LM3 depend on the requirements of the client (model) processes (*e.g.*, land use/cover, grouping of *Receptors* for scale-dependent risk characterisation, weather, soil, etc.). LM3 for exposure calculation: The agricultural field represents the basic exposure source unit from which substances can expose surrounding habitats; a source-centred topological data model should be considered. Exposure routes for spray-drift and run-off should be considered with the option to add further routes.
Flexibility, Extensibility,	Generic approach with respect to habitat types of Non-Target-Organisms (*e.g.*, terrestric and aquatic). Flexible and extendable approach in order to enable

Topic	Aspect
Scalability	the use of different geodata and to parameterise different exposure, eFate and effect models which run within the Xplicit approach (Section 5.3.4). The landscape-metric generation should be scalable, *i.e.,* applicable to a range of study region (landscape) extents. To this end, the study region should be divided into sub-regions which are subject to parallel processing.
System, Technology, Implementation	Modular system distinguishing between geoprocessing and non-geoprocessing modules (which may be running at different machines), including, *e.g.,* GIS data processing module, topology generation logic module and service endpoint. Usage of common technologies provided by ArcGIS (desktop, server), Microsoft.NET, RDBMS, file services, (http). Basic modules: GIS processing, .NET software, data service endpoint. ArcGIS toolbox modules (using the ArcGIS model builder), including standard tools and own developments (ArcGIS, .NET, Python). LM3 generator as C# .NET software, with key module (class) 'LM3-Service'. 'LM3-Service': Core LM3 data service module (class) which defines the functionality the LM3 has to provide. The main LM3 clients are the geoprocess (during LM3 generation) and the landscape-scale RA model (Xplicit, *XE*, *XA*, Section 5.3.4).

Architecture and System Design

This section introduces major elements of the LM3 architecture and system design as developed following the objectives and requirements (Table 7). Figure 24 provides an illustration of the LM3 modules and their interaction.

The LM3 can be regarded as an interpreter (Figure 25) that transforms geographic entities as provided in base geodata (*e.g.,* land use/cover; their type, location and attributes) into objects and their relationships relevant to landscape-scale modelling (Xplicit). The LM3 discretises and transforms objects from the geographic space into a topological modelling space.

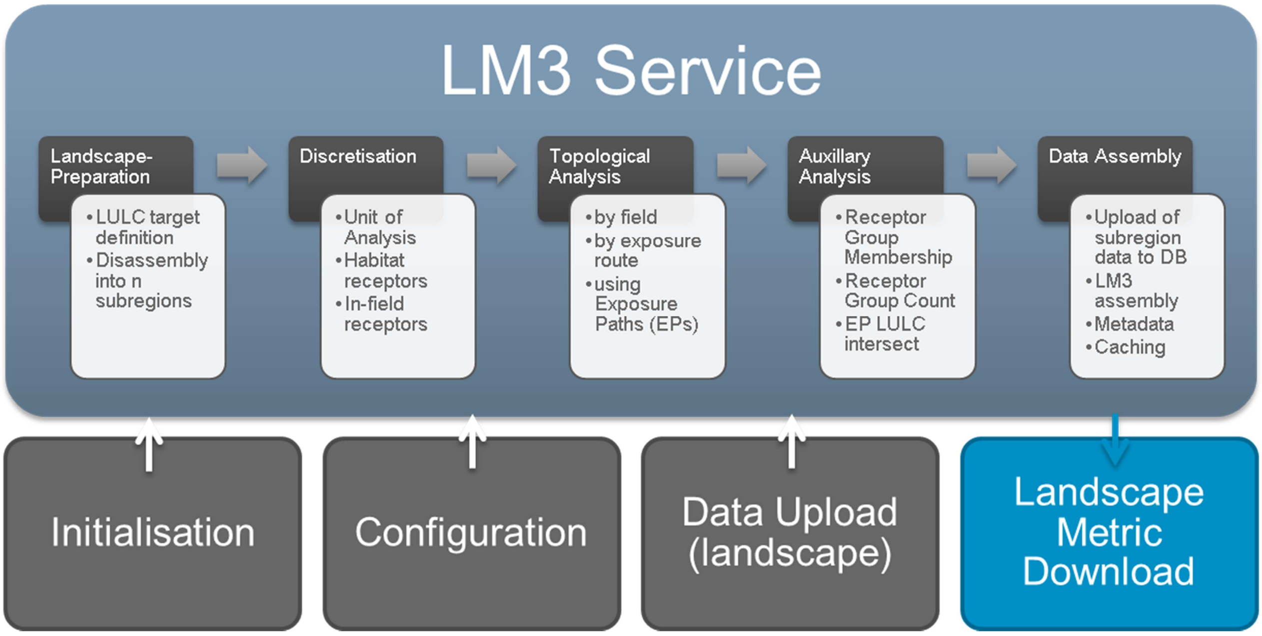


Figure 24: *Landscape-Metric* service (version 3, 'LM3') modules and process (LULC = land use / land cover).

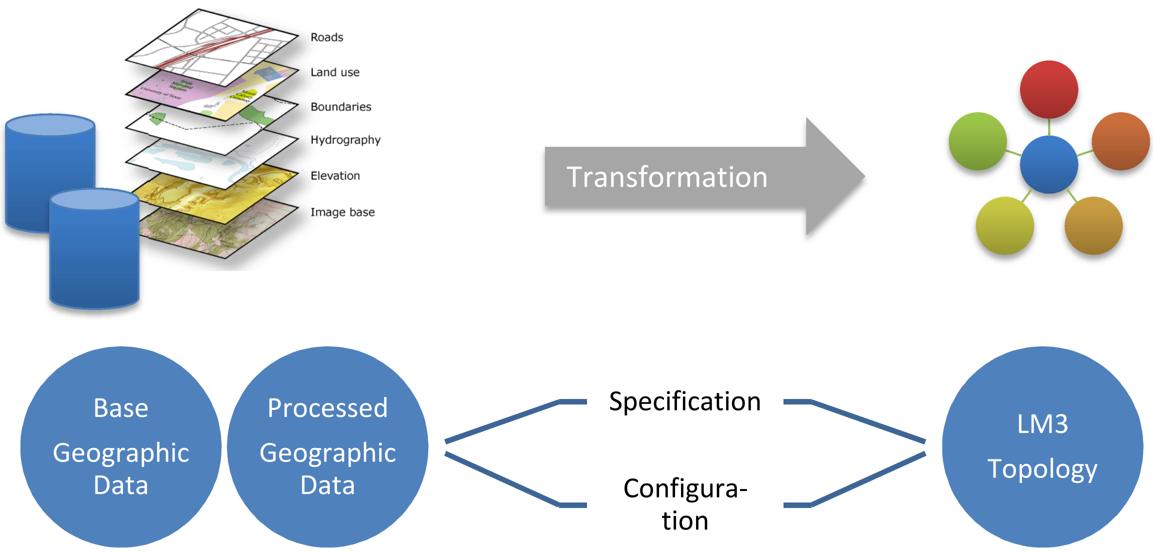


Figure 25: Geodata transformation, from the geographic space into the object relationship space (topology). (GIS layer graphic: ESRI 2012).

The landscape-scale modelling, together with a RA problem formulation, determines the definition of the LM3 structure and content, and, so, the geodata processing steps. Depending on the availability of adequate base geodata, the RA problem formulation can also influence geodata development. Ideally, landscape-scale risk characterisation modelling largely makes use of readily available base geodata. Base geodata can range from common topographic maps to geodata specifically developed according to a RA problem formulation.

Receptors represent the smallest spatial unit of analysis in the Xplicit approach (Section 5.3.4.9). They are the result of geodata discretisation. The approach distinguishes *In-field-Receptor* and *Off-Crop-Receptors* (Section 5.3.4.9).

In-field-Receptors are located on target crop fields. As PPPs are applied on fields, the field is regarded the primary exposure unit. They directly receive substances from PPP application. Depending on the exposure route and the related model approach, they are either placed equidistantly on a target field's boundary line (*e.g.*, for spray-drift modelling) or as grid on the target field's surface (*e.g.*, for run-off modelling).

Off-Crop-Receptors represent segments of basically any habitat type of Non-Target-Organisms (*e.g.*, terrestric, aquatic). Usually they are placed as one or two dimensional grids onto off-crop surfaces (Figure 26), which can be represented as line (*e.g.*, a stream) or polygon (*e.g.*, a grove, herbaceous polygon). *Receptors* can take all thematic data from the geodata entities at which they are placed. Further characteristics and behaviour of receptors is discussed in Section 5.3.4.9. Receptor spacing is determined by the RA problem formulation and is configured by the user (independently for *In-field-* and *Off-Crop-Receptors*).

Each *Receptor* obtains a unique identifier which persists throughout the process 'from geodata to LM3'. It links the LM3 entity 'receptor' to the geodata point, and thus, allows to map Xplicit simulation and evaluation (*XA*) outcome back to the geodata.

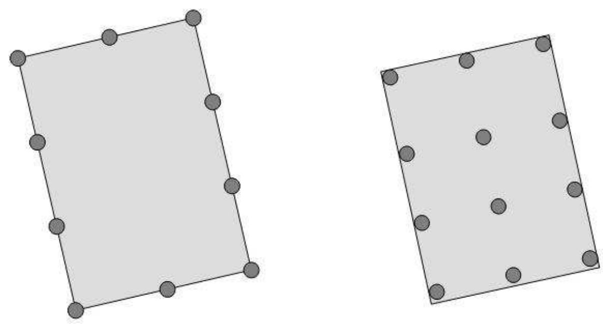


Figure 26: Illustration of *In-field-Receptor*; here, placed onto field boundary (left) or as grid onto field area (right).

Exposure Paths (EPs) are trajectories which determine the paths that substances take. Like *Receptors*, EPs represent a base topological element. EPs are determined on the basis of *Receptors* (above). As the agricultural field is the base unit of farmer activity, including the use of PPPs, EPs typically start at *In-field-Receptor*. EPs can basically represent any exposure type and route, hence, the shape of an EP can be a straight line or form a more complex trajectory, depending on the type of exposure modelled: *e.g.*, spray-drift, dry-deposition, run-off, dust-drift. Starting from an *In-field-Receptor*, EPs extend into the landscape, *e.g.*, up to a predefined distance at which the level of exposure is regarded irrelevant (Figure 28) or up to a specific land use/land cover type (*e.g.*, water body, Figure 29).

The topological relationship of *In-field-Receptors* and *Off-Crop-Receptors* (Section 5.3.4) is established by allocating *Off-Crop-Receptors* to neighbouring EPs (Figure 27). Visually speaking, along their extent, EPs 'collect' *Off-Crop-Receptors* located in their vicinity. All relevant data for parameterising a predefined local exposure model are recorded (*e.g.*, distance from *In-field-Receptor* to *Off-Crop-Receptor* and intersected land cover).

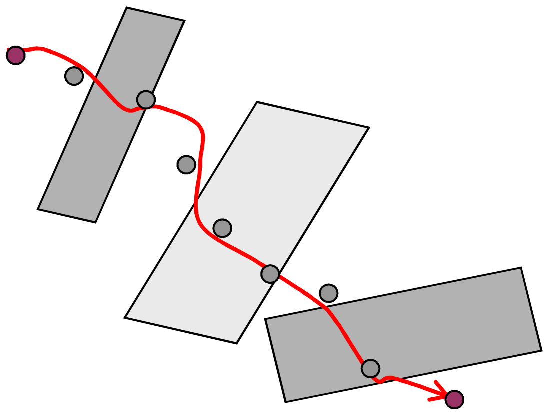


Figure 27: An EP starting at an *In-field-Receptor*, allocated *Off-Crop-Receptors* and intersected land use/cover (grey areas).

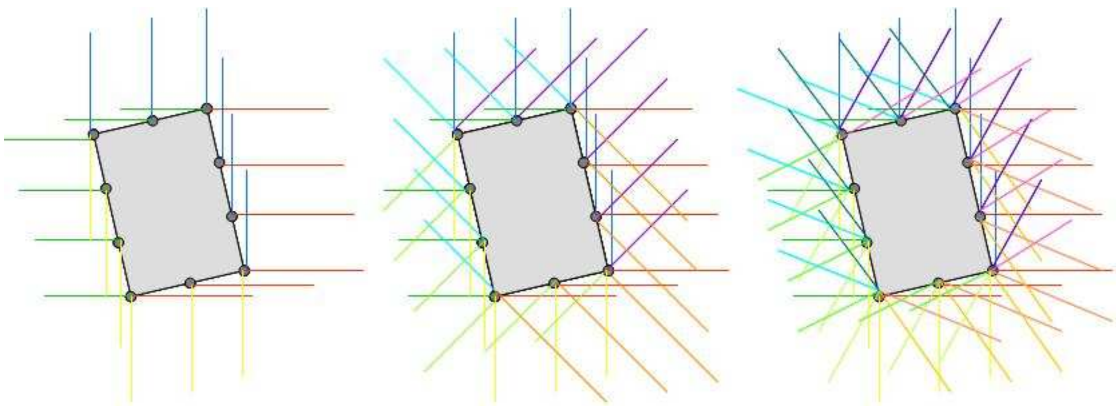


Figure 28: EPs representing spray-drift for discretised wind directions (see also Figure 31). Equispaced directions can be chosen (*e.g.,* 4, 8, 12). (grey dots = *In-field-Receptor*, no *Off-Crop-Receptors* shown.)

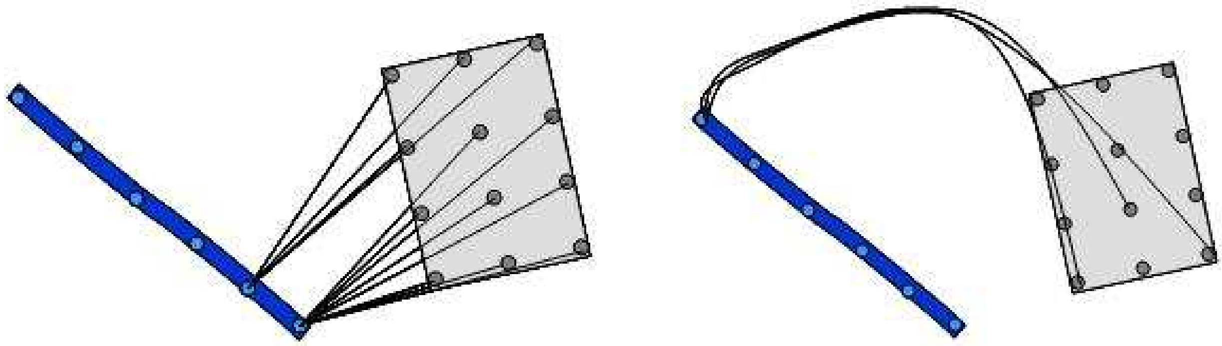


Figure 29: EPs representing run-off. The current LM3 version allows to choose either the shortest connection (left) between an *In-field-Receptor* (grey dots) and an *Off-Crop-Receptor* (blue dot, representing a water body segment), or – if a digital elevation model is available – an EP that follows the surface slope (right).

A *Landscape-Metric* service has to represent the relevant data for specific landscape-scale RA modelling. Study problem formulation and design (*e.g.*, exposure and eFate models used) determine the data content and structure that is to be provided by the *Landscape-Metric*. Data organisation in different related tables follows database normalisation requirements (*e.g.*, Schäfer 2010).

Landscape-Metric services realised in version LM3 are capable to provide data for characterising abiotic *Receptors* in the context of spray-drift and run-off exposure modelling, for simple eFate modelling (*e.g.*, dissipation) and for scale-dependent analysis of *Xplicit-Model* outcome (*XA*, Section 5.3.4.4). *E.g.*, the LM3 contains the following tables to parameterise a risk characterisation study for aquatic plants due to spray-drift (case study, Section 6.3):

- *Receptor-table*: lists all *In-field-Receptors* and typically a sub-sample of all *Off-Crop-Receptors* occurring in a study region, excluding *Off-Crop-Receptors* for which exposure is unlikely due to their distance to fields. For efficiency reasons, such *Receptors* are excluded from modelling. However, the existence of these *Receptors* can be relevant to ecological risk characterisation and RM. Therefore, the occurrence (counts) of these *Receptors* is registered in the *ReceptorGroupCount-table* (below). A LULC ID column relates a receptor to the land use/cover it represents (below). Additional attributes (columns) can be added in the LM generation process (or in a subsequent extension) and allow to characterise environmental conditions (*e.g.*, soil types, weather zones) or to assign *Receptors* to certain groups. In the example, in which *Receptors* represent water body segments, *Receptors* are grouped by individual water body as well as by distance from PPP use areas (rails). At minimum, two groups are predefined, the 'receptor-group', in which each individual *Receptor* build its own group (predefined group-type = 0) and the 'SR-group', a single group representing the entire study region (predefined group-type = 99).
- *Exposure-Path-table*: The LM3 employs a source-centred perspective to exposure modelling in which *In-field-Receptors* are initially exposed and so build the source of potential exposure of *Off-Crop-Receptors*. Correspondingly, EPs for spray-drift start at

an *In-field-Receptor* and extend into the landscape up to a predefined length. The spray-drift exposure model used in the example is based on the downwind *In-field-Receptor*–to–*Off-Crop-Receptor* distance. As shown above, potential wind directions are discretised, hence, distances are quantified in predefined directions. Therefore, the EP-table for spray-drift contains distance records for each *In-field-Receptor* and each possible wind direction. Each record thereby consists of a tupel of '(receptor-ID,distance[m])'-pairs. Likewise, each EP records a tupel of '(LULC-type-ID,from-distance,to-distance [m])'-triplicates, representing land cover types intersected by the according EP (in the example, to parameterise spray-drift filtering of intervening vegetation).

- *LULC-table*: Data (*e.g.*, descriptive) on LULC-types (land use/cover) relevant for *Receptor* characterisation.
- *ReceptorGroupCount-table*: As discussed above the *Receptors-table* typically contains only a sub-sample of all *Off-Crop-Receptors* occurring in a study region for efficiency reasons. The *ReceptorGroupCount-table* counts the total number of *Off-Crop-Receptors* by group (including the receptors listed in the receptor-table).
- *ReceptorGroupTypes-table*: Receptor group type identifiers.
- *Metadata-table*: Following the requirement that each *Landscape-Metric* characterises itself, metadata is provided for each LM3. The metadata basically describes the parameters and conditions of the LM3-generation process (XML-data, user, date, etc.).

Depending on the study design, the *Landscape-Metric* data content and structure might be adapted and extended by further data (tables).

GIS-tools, including Model Builder-Tools and Python scripts (ArcGIS desktop and server, ESRI 2012) and Microsoft .NET classes (Microsoft 2012b, C#) were developed in order to provide the LM3 generation functionality. For the EP spatial analysis step (spray-drift) a .NET module had to be developed which was then integrated into the GIS-toolbox and processing sequence (due to unreasonable processing costs using standard GIS-tools). Currently, the *Landscape-Metric* version 3 ('LM3') is physically stored in a local or central database (e.g. ORACLE, or in off-premises cloud storages, *e.g.*, Microsoft Azure (Microsoft 2013)), or, alternatively, as binary files on network file drives. Currently, the database is the usually used main *Landscape-Metric* access endpoint 'on-premises'.

The field represents the base unit of analysis throughout the *Landscape-Metric* generation process which allows for parallel computing. Concepts include a central .NET module, 'LM3-Service', as the single processing access endpoint. The LM3-Service controls the entire LM3 generation process, including landscape split into sub-SRs, their parallel processing, metadata generation, and subsequent compilation (Figure 33). Metadata is accessed by Xplicit-Models.

LM3 generation tools comprise modules for general process control (Figure 30), as well as modules for the transformation of geodata to topological data (the actual *Landscape-Metric*, examples, Section 6). Concepts and their implementation take a future extension of the specific functionality into account.

LM3 Generation Process

The general LM3 generation sequence is illustrated in Figure 30 (next page). The process starts with geodata preparation using GIS. Configuration and actual processing supervision is done by the LM3-Service, which especially manages study region splitting and parallel processing of sub-regions. The latter assures LM3 service scalability.

As of this writing, the key processing steps have been implemented, yet, some automation steps are still under development. Also, some modules are implemented with basic functionality only and have to be extended with further development (*e.g.*, rules in quality check). The *Receptor*-grouping step is optional and can be added any time.

Like the data that is to be provided by a *Landscape-Metric*, the LM3 generation process is guided by the study definition (*e.g.*, problem formulation, Assessment Endpoints, scales, exposure model(s), input geodata, etc.). Study regions can range from the vicinity of a single field (*e.g.*, single edge-of-the-field-scale risk characterisation) to some ten or hundred thousands of hectares.

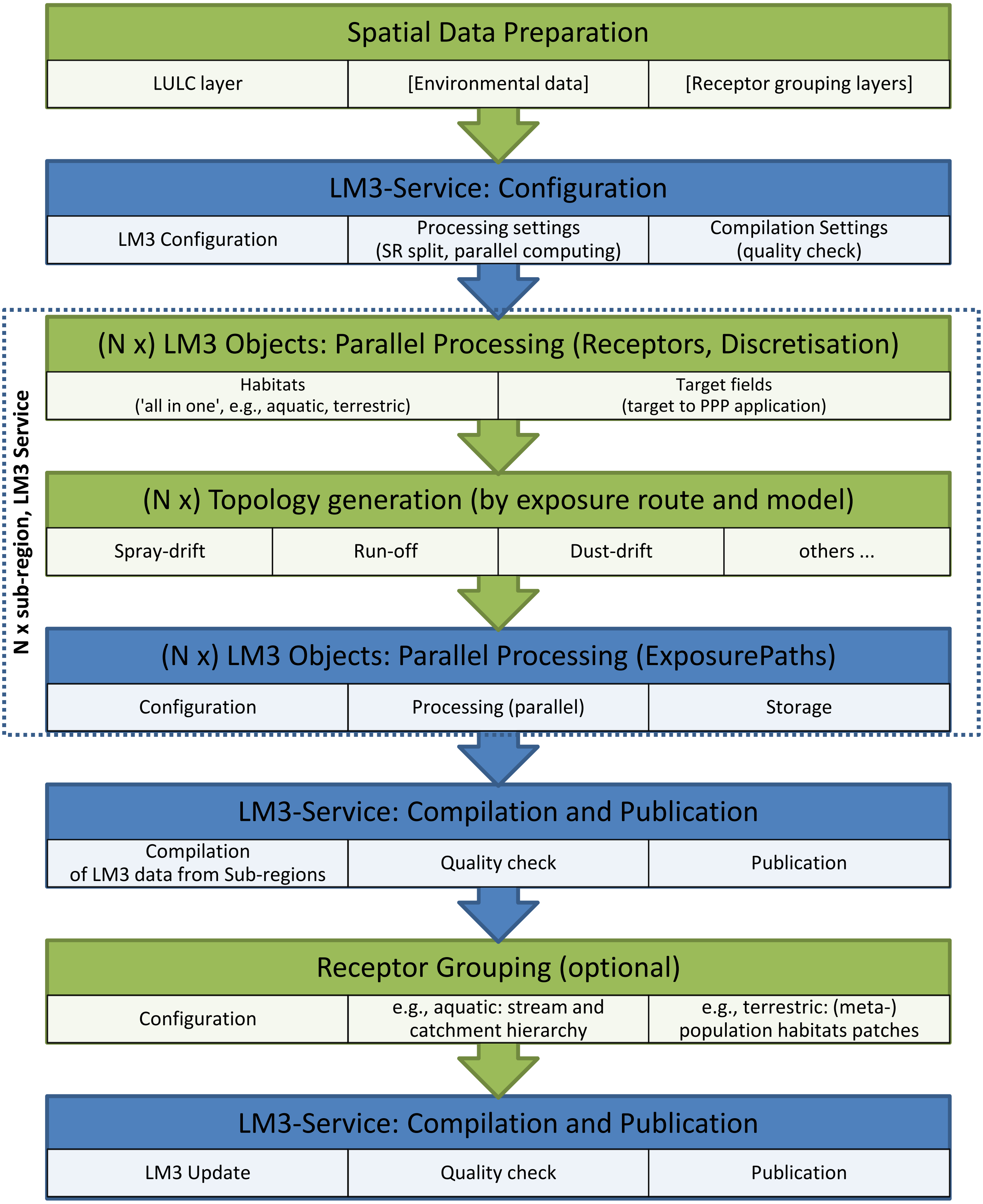


Figure 30: LM3 generation process steps and modules (green: GIS process, blue: .NET module, SR = study region, elements in '[]' are optional).

5.3.5.3 Modelling Exposure Due to Spray-drift – Problem Definition

Spray application of PPPs generally is accompanied by a certain fraction of the spray volume leaving the targeted field and depositing into neighbouring habitats of Non-Target-Organisms. The mechanistic process of spray droplets movement - from leaving the nozzle, their trajectory through the air and their deposition onto habitat elements - is complex. Therefore, with the aim to establish a robust basis for ecological RA and RM in the authorisation of PPPs, estimation of spray-drift depositions is currently predominately approached empirically (mechanistic approaches are in early use stages in regulatory RA and RM, *e.g.*, Holterman *et al.* 1997, Miller & Hadfield 1989, Endalewa *et al.* 2010). Ganzelmeier *et al.* (1995) and Rautmann *et al.* (2001) provided a collection and evaluation of spray-drift experiments which established an empirical exposure modelling approach due to spray-drift (*e.g.*, FOCUS 2001). In this approach, spray-drift depositions onto habitats of Non-Target-Organisms occurring at the edge-of-the-field are basically represented by the 90th percentile depositions observed within and between field trials (at a given field-to-habitat distance). The variability occurring along the field edge (at a given distance) or between different applications is ignored. However, this variability can represent an important landscape factor in ecological risk characterisation, taking different landscape scales into account (*e.g.*, Schad & Schulz 2011).

Spray-drift deposition data underlying the evaluation of Rautmann *et al.* (2001) were analysed in a Bayer CropScience study ("*Empirical Models of Spray-drift Variability for Landscape-scale Exposure and Risk Assessment*", Schad & Gao 2011, Bayer CropScience, unpublished) with the aim to develop spray-drift deposition PDFs which sufficiently represent variability of spray-drift depositions in field vicinity and which are applicable in the Xplicit approach (Section 5.3.5.4).

In Figure 31, scales and their hierarchical relationship are illustrated as defined for spray-drift calculations in the Xplicit approach. The scales and their relationship were defined on the background of spatial units already defined in the Xplicit approach (*e.g.*, *Receptors* representing the smallest unit-of-analysis, fields as the unit of PPP application, *Exposure-Paths* (Section 5.3.5.2)) and the design of spray-drift experiments (*e.g.*, interval of spray-drift deposition measurements along the field boundary, Section 5.3.5.4).

The amount of spray-drift reaching a local habitat segment of Non-Target-Organisms depends further on the occurrence of spray-drift filtering landscape elements located between the sprayed field and the habitat. In Section 5.3.5.5, the results of a literature review are presented which aimed at the characterisation of the spray-drift filter effect of (riparian) vegetation (Schad T, Ohliger R, Schulz R, 2009, Bayer CropScience, unpublished).

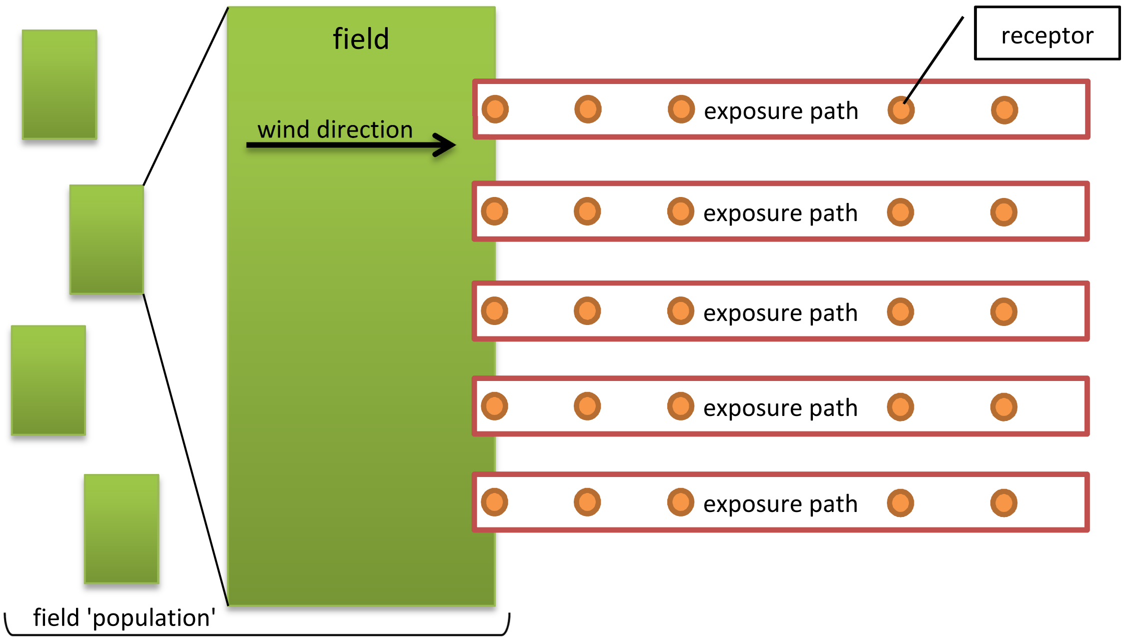


Figure 31: Scales in exposure due to spray-drift deposition: 'population' of fields, field, exposure path (EP), *Receptor*. *In-field-Receptors* located at the field boundary are considered as primary sources of spray-drift exposure along the exposure paths.

5.3.5.4 Modelling Exposure Due to Spray-drift – 'Schad & Gao' Approach

5.3.5.4.1 Abstract

The objective of the present analysis was to develop empirical spray-drift deposition models applicable in landscape-scale ERA, based on the data underlying the official 'Abdrifteckwerte' (Rautmann *et al.* 2001, crop types 'arable', 'hops', 'orchards-late', 'orchards-early', 'vines'). The models are represented by Probability Density Functions (PDFs). In landscape-scale risk characterisation, scale dependencies of variability have to be taken into account in order to assess conditions that can occur in the real-world. In the case of spray-drift deposition, it has to be evaluated, *e.g.*, which variability can be assigned to a spray event of a certain field, or how to correlate spray-drift depositions occurring along a drift swath (of about 1-10 m width).

Empirical models (PDFs) were developed that allow to represent the variability of spray-drift deposition underlying the official 'Abdrifteckwerte', adequate for landscape-scale ERA. The results provide the study director of a landscape-scale approach with the possibility to employ different empirical models, *e.g.*, depending on the scale at which spray-drift variability is to be represented or the scale of the aggregation of the outcome of the ERA (*e.g.*, local or regional).

Five approaches were employed to develop PDFs (by crop type and distance to field edge). The results of approaches (i)-(iii) are recommended to be used in landscape-scale ERA and represent different levels of trial-grouping. The results of approach (v) demonstrate a methodology to refine the representation of correlations along a drift swath:

i. **'Individual-trial-analysis'**: uniform, normal, lognormal, gamma and beta distributions were fitted to spray-drift depositions of individual trials. Uniform PDFs are recommended to be used in landscape-scale ERA, in which in a 1st step, a trial (or its conditions) are randomly determined and then, in a 2nd step, the PDF is sampled.

ii. **'Lumped-analysis'**: all trials of a crop type were pooled. Among the distributions fitted, gamma performed best; however, also other distributions resulted in statistically significant results. For the use in landscape-scale studies, a justification for representing all variability in a single PDF should be considered (*e.g.*, especially regarding agricultural conditions).

iii. **'*A priori* grouping'**: Trials of a crop type were assigned into predefined groups, determined by expert judgement (depending on trial conditions 'wind speed', 'pressure' and 'spraying technology'). For each group, the same analysis was performed as for the 'Lumped-analysis'. Statistically significant results were obtained for different distributions. Again, gamma performed best. The results can be used in two ways in landscape-scale ERA: (a) 'by group' (recommended), *i.e.,* 1st sampling a group (according to the conditions it represents) and then, 2nd, sampling the PDF of this group; (b) 'Lumped-analysis-2', which provides a linear combination of the PDFs (by crop type and distance), that can be regarded as an improved fit to the pooled variability of all trials of a crop type (and distance), compared to the 'Lumped-analysis'. Again, the gamma distribution fitted best but other distributions can be used as well.

iv. **'Automated trial grouping'**: In contrast to the '*a priori*' approach, the goal of the 'automated trial grouping' was to determine trial groups by statistical means. A small number of groups were intended to be obtained. Different approaches were applied to 'automatically' determine trial groups and to assign the individual trials to them (*e.g.*, Cluster Analysis, Tree Regression Analysis). Due to the basically complex nature to which extent the different parameters (*e.g.*, wind conditions, pressure) affected local spray-drift deposition, automated grouping of trials by statistical means did not result in outcome that could reliably be used in landscape-scale ERA.

v. **'Mixed-effect-model'**: Independent sampling for each distance from the field suffers from the shortcoming that it may generate non-sensible results along an exposure path (swath), like a very low deposition at close distances but a high deposition at farther distances. This problem can be solved by sampling the quantile first for an exposure path and then use this quantile of the fitted distributions at each distance as the sampled value. This preserves the general trend over the distances. However, the observed variability along the exposure path is lost (corresponds to 100% correlation along the swath). Instead, an overall probabilistic distribution for all the data in all distances and trials can be used to account for the trend that the drift deposition decreases as the distance increases while keeping both the in-swath and between-swath variability. A Mixed-effect model is suitable for this purpose. Different trials are considered as a categorical covariate representing “experimental units” in the deposition data set since the experimental conditions are similar for one trial but vary considerably across different trials.

Due to the complexity, neither the autocorrelation in one swath along the distance nor the correlation within one trial among swaths is considered in this modelling approach. Except for distance, other covariates were not included as predictors. Further work in the direction may improve the model.

This approach usually produces higher percentiles compared to previous approaches. One reason is that two levels of variability are present in this model, which makes the overall distribution broader. Moreover, the regression is done on the log of the observed values and log of the distances, which can cause extremely large predictions of the deposition at the small distances.

However, this modelling approach shows a promising perspective for developing a comprehensive analysis framework by deriving an overall PDF and making scale-dependent predictions of future events based on that.

5.3.5.4.2 Introduction and Objective

Risk for Non-Target-Organisms to be adversely affected by PPPs is supposed to be largely driven by spatial and temporal variability (*e.g.*, Verdonck 2003) of environmental, ecological and agricultural conditions (*e.g.*, composition and structure of landscape, species occurrence and life cycle, stochasticity of application or weather events).

Spray-drift is regarded a major exposure route to habitats of Non-Target-Species (terrestrial, aquatic) as considerable fractions of the amount of PPP applied can drift across the field boundary and deposit in the vicinity. Spray-drift deposition was measured in a number of field trials (Ganzelmeier *et al.* 1995, Rautmann *et al.* 2001) which were statistically evaluated to derive 90th percentile depositions for certain distances from the field. These deterministic values build the basis of the standard exposure scenarios for spray-drift ('Tier-1' scenario) as part of the ecological RA in the European Union and its Member States.

In contrast to the Tier-1 scenario, landscape-scale risk characterisation needs to take local variability of exposure-driving factors, *e.g.*, of spray-drift deposition, into account in order to produce reasonable results (Schad & Schulz 2011).

Being deterministic, the standard scenarios for exposure due to spray-drift ignore variability of spray-drift depositions, whereas variability of measured deposition is substantial (Rautmann *et al.* 2001). Statistical evaluations to describe this variability were done by Strassemeyer (JKI, 2008, pers. comm.), Wang and Rautmann (2008) and Golla *et al.* (2011).

In the analysis of Golla *et al.* (2011) and Strassemeyer (JKI, 2008, pers. comm.), the arithmetic mean of samples of each distance and trial were calculated, and these arithmetic means of all trials of a certain crop type (hops, orchards-early, orchards-late, vines, arable) for each distance were pooled. Resulting Probability Density Functions (PDFs) therefore represent spray-drift variability of the mean deposition for each measured distances of all trials of a crop type (herein called 'lumped analysis'). Normal distributions were fitted to the data. The authors justify the use of the mean deposition by referring to the proposed application of the PDFs for landscape-scale aquatic exposure assessment, assuming that small-scale variability will average out in the water body. There was no justification or evaluation given for the pooling of all trials of a crop type into a single PDF (for each distance). This has the consequence that even the agricultural conditions (*e.g.*, nozzle type, pressure) effectively vary from sample to sample drawn from the PDF, which could cause unrealistic deposition patterns next to a single field in landscape-scale RA. In other words, potential differences in within-trial to between-trial variability were not evaluated.

The latter considerations were also undertaken in the evaluation of spray-drift variability by Wang & Rautmann (2008), which concluded to derive PDFs for each individual trial (herein called 'individual trial analysis'). The analysis was focused on orchards. In their landscape-scale exposure assessment model, exposure next to a field at which a spray application was performed was calculated by, first, randomly selecting a trial, and second, by sampling the (distance-dependent) PDF of this trial. This approach, however, assumes, on one hand, that relevant conditions between trials are significantly larger that than those within trial (so, ignoring other trial data to assess a single application), that conditions of a single trial can be assigned to a certain spray event in the model, and that the range of such conditions occur in the investigated landscape. Moreover, the authors fitted gamma distributions to the single trial deposition data without providing quantitative justification for choosing this distribution. This needs to be questioned due to the small sample size of measured spray-drift deposition for the individual distances, which is typically around six data points.

In a previous analysis step, Wang & Rautmann (2008) evaluated trial conditions (environmental, agricultural) for their contribution to spray-drift deposition. In summary, spray-drift deposition was most sensitive to wind speed, spray pressure and nozzle type (as well as relative humidity).

The analysis presented herein followed the key objective to derive PDFs, together with recommendation on their use, in order to sufficiently address variability of spray-drift depositions close to treated fields in landscape-scale risk characterisation.

5.3.5.4.3 Data and Methods

The analysis was based on the trials underlying the official 'Abdrifteckwerte' (Rautmann *et al.* 2001). Therefore, the same trial data were applied as used in the definition of the standard spray-drift scenario. Data were neither neglected nor added.

Standard Scenario

The standard scenario for exposure due to spray-drift assumes the occurrence of the habitat of the Non-Target-Species downwind and in close vicinity to the treated field (Rautmann *et al.* 2001). For each crop and measured distance, a 90th percentile spray-drift deposition was derived (detailed methodology in Rautmann *et al.* 2001). Values are expressed in '% of application rate'.

Data and Data Preparation

Measured data on spray-drift deposition underlying the official 'Abdrifteckwerte' (Rautmann *et al.* 2001) were kindly provided by Rautmann (Julius Kühn Institute, 2010, *via* email from 21 July 2010).

Spray-drift deposition was measured typically at distances 3, 5, 10, 15, 20, 30, 50 m (for arable also at 1 m, in some trials also at 7.5 m distance and at distances >50 m, up to 100 m). At each distance, up to 10 samples were taken (on average about 6 samples). The samples represent the intra-trial variability, whereas samples of different trials also represent inter-trial variability.

Data preparation: Missing data (*e.g.*, trial '99', vines, no data for distances >20 m) were omitted in the analysis. The smallest data value of a trial was regarded as the limit of detection (LOD, *e.g.*, 0.01 % in trial '222', arable) and was used to replace '0' values by ½ the LOD. For arable, measurements at '0 m' distance were not taken into account as habitats of off-crop Non-Target-Species are not considered to occur at 0 m distance and as overspray of habitats does not comply with Good Agricultural Practise and hence, is not considered relevant in the ecological RA.

Total number of trials: hops (21), orchards-late (30), orchards-early (41), vines (21), arable (58).

Individual Trial Analysis

The goal of the individual trial analysis was to derive PDFs for each measured distance of each individual trial and thereby to evaluate whether a certain PDF type fits the data best.

In a landscape-scale ERA, a trial is randomly selected to represent spray-drift of a field that is applied by spray application in the model, *i.e.*, in the landscape-scale model it is assumed that environmental and agricultural conditions are prevailing as in the selected trial. For further fields in the model, new random selections are performed. In case knowledge on *e.g.*, the distribution of a certain spray technology in a region is available, this data can be used in the random selection of trials.

For each individual trial, five different distribution types were fitted to the data: uniform, normal, lognormal, gamma, and beta.

In general, there are only 4-6 measurements, at most 10, at each distance in each trial. With this small number of data points, it is very hard to determine the kind of distribution from which the drift measurements come from. For example, the p-values of Kolmogorov-Smirnov test are in general far greater than 0.05, suggesting that there is no evidence to reject any type of the distributions. For distances with '0' measurements, no gamma was calculated. For distances with very low variability (mostly at larger distances), also no gamma was calculated.

The uniform distribution as the most simple of the considered distributions (regarding the assumptions made) is probably good enough for sampling purposes, with the drawback of not being able to sample drifts higher than the maximum observed ones or lower than the minimum observed ones.

Lumped Analysis

The goal of the lumped analysis was to derive a single PDF for each crop type and distance representing the entire variability observed within the spray-drift deposition measurements.

In landscape-scale ERA, the use of a lumped PDF is justified *e.g.*, if inter-trial variability is not significantly larger than intra-trial, or if results of calculations at local-scale are aggregated at larger scales (*e.g.*, regional scale). Descriptively speaking, the use of a lumped PDF is justified, if agricultural (*e.g.*, nozzle type, pressure) and field-scale environmental conditions contribute less to local variability of spray-drift depositions than within-field small-scale factors (*e.g.*, crop canopy density, locally varying wind speeds and turbulences).

The lumped analysis was done by fitting a distribution to the data after pooling all the trials (by crop type). Four kinds of distributions were fitted: normal, lognormal, gamma and beta.

The p-values and the test statistics of the Kolmogorov-Smirnov test were examined. Also, the BIC values (Bayes Information Criterion) were compared. A p-value smaller than 0.05 indicates that the fitted distribution should be rejected at the 95% confidence level. The smaller the test-statistic, the closer is the distance between the empirical CDF (Cumulative Distribution Function) from the data and the fitted distribution CDF. The smaller the BIC, the better the distribution fits the data.

For hops, two trials were found to show significantly lower deposition than the others (Trial 116, 117). This observation could not be adequately represented by the distribution fits. Therefore, for hops a 'lumped-level2' analysis was performed without Trial 116 and 117, which resulted in conservative PDFs with respect to landscape-scale ERA.

Subsequent to distribution fitting, a regression analysis on the fitted distribution parameters against the corresponding distances was performed. The results allow to use the PDFs in landscape-scale approaches at distances different from the distances measured in the trials (interpolation).

Two alternatives regression functions were tested (Equation 3, Equation 4):

Equation 3: $\ln(\mu) = a + b \bullet \ln(x)$; x = distance [m]; a, b = regression parameter ([-])

Equation 4: $\ln(\mu) = a + b \bullet x$; x = distance [m]; a, b = regression parameter (b: [1/m])

Grouped Analysis

Spray-drift deposition trials were conducted at different agricultural (*e.g.*, nozzle type, pressure) and variable environmental (*e.g.*, wind speed variability) conditions (Rautmann *et al.* 2001), which could have caused significant differences in spray-drift depositions between the trials (inter-trial variability). Consequently, spray-drift variability next to a treated field could be better represented by a certain group of trials, which are characterised by certain agricultural and environmental conditions, than by a lumped distribution representing all trials for a crop.

Wang & Rautmann (2008) found that nozzle type, pressure and wind speed significantly affected spray-drift deposition. Therefore, in a first approach, trials were *a priori* grouped in pre-defined categories of these three trial conditions. In a second approach, attempts were made to derive groups of trials by statistical means.

A priori Trial Grouping

Among environmental conditions affecting spray-drift deposition, wind direction and wind speed are most prominent (*e.g.*, Wang & Rautmann 2008, Rautmann pers. comm. 2008). Spray-drift deposition obviously occurs downwind from a sprayed field. Even though the effect of wind speed on the spray-drift deposition at different distances can be quite complex (*e.g.*, Wang & Rautmann 2008), in the range of wind speeds that allow spraying in the framework of Good Agricultural Practice, one can state that as a general trend, the higher the wind speed, the higher the deposition. Among agricultural conditions affecting spray-drift deposition, nozzle type and pressure are also prominent (*e.g.*, Wang & Rautmann 2008, Rautmann pers. comm. 2008).

The distribution of wind speed, pressure and technology were used to *a priori* categorise trials into groups (by crop type). Technology is a lumped parameter derived from nozzle and machinery type. The approach aimed at grouping trials into a few groups by expert knowledge and by using the frequency distribution of the three parameters in focus (*e.g.*, range, modes, percentiles, outliers, *etc.*). Categorisation of trials by different nozzle types and spraying technology was done in consultation of experts (D. Rautmann 2010, pers. comm., and A.C. Chapple 2010, pers. comm.).

In Table 8, a summary is given of the resulting group boundaries of the individual parameters and the effective total number of groups.

Table 8: Trial group boundaries for conditions 'wind speed' and 'pressure', 'technology', as well as total number ('#') of resulting groups (boundary value is included in the lower bin, *i.e.,* defines the upper value of the lower bin).

Crop Type	**Wind-speed [m/s]**	**Pressure [bar]**	**Technology (# groups)**	**Effective Total # of Groups$^{\Delta}$**
Arable	3	3.5	4	7
Hops	0.5, 2.5	20	2	4
Orchards-late	1.5	10	4	7
Orchards-early	1.5 , 4.5	3	1	4
Vines	1.6	-	2	3

$^{\Delta}$ as effectively realised combinations in the trials

Each group represents a certain combination of (environmental and agricultural) conditions prevailing during spray application. For each group (of each crop type), PDFs were fitted to the deposition data (of the different distances). The result can be used in landscape-scale ERA as follows:

- **'Condition Group'**: In landscape-scale ERA, certain conditions can be assumed to prevail during an individual application (or *e.g.*, for a number of applications in a spatiotemporal scale). A group will be (randomly) selected according to the prevailing conditions (wind speed range, nozzle/pressure range). Data on wind conditions and the distribution of spraying technology can be used to define the frequency of group occurrence in a study region.
- **'Lumped Analysis 2'**: In case the *a priori* grouping approach resulted in improved distribution fitting compared to the all trials including 'Lumped Analysis' (above), a linear combination of the PDFs obtained for the individual groups (of a crop type) can be derived representing an improved 'Lumped Analysis 2', *i.e.,* the overall distribution can be seen as a mixture of *e.g.*, normal or gamma distributions. An example is plotted in Figure 32.

The difference between the conditions and the a priori groups was compared *via* a Tukey's honest significance test. The test compares the means of drift residue in every condition to the means in every other condition. It is essentially a modified t-test for doing multiple comparisons in one-step. The intervals are calculated based on the range of sample means and studentized range statistics rather that pair wise individual differences and t-distribution. Therefore it will not inflate the probability of declaring a significant difference when it is not present.

Designation and characterisation of *a priori* groups is shown in Table A 4 in Appendix 11.3.1 (as effectively resulting from the conditions that occurred in the measurements).

For each group a normal and gamma distribution was fitted to the drift residue data, so that the overall distribution can be seen as a mixture of normal or gamma, if the combination of conditions in the experiments is considered as a random sample.

Suppose there are n *a priori* groups: the probability distribution function can then be written as follows:

Equation 5

$$p(y) = \sum_{i=1}^{n} \pi_i p(y_i)$$

where *y* is the vector of observed drift residue, and y_i is the vector of drifts in the ith group. Assuming a normal distribution for each group, then it follows that:

Equation 6

$$p(y_i) = \prod_{j=1}^{n_i} \frac{1}{\sqrt{2\pi_i}\sigma_i} \exp\left\{ \frac{(y_{ij} - \mu_i)^2}{2\sigma_i^{\,2}} \right\}$$

It should be noted that this mixture of normal was not estimated directly since each trial was pre-labelled into a group already defined. Instead, π_i was simply estimated by the percentage of trials which belongs to the ith group, and the μ_i and σ_i by the mean and standard deviation of the drift measurements in the ith group.

In this way, the fitted distributions can capture both the heavy tails and the additional peaks in the low value regions that occur often in the data.

In landscape-scale ERA, the fitted 'mixed' distributions (PDFs) can be used as a probabilistic spray drift model just as a simple distribution (as proposed for the 'Lumped Analysis', above). For any given distance from fields, the environmental and technical conditions need to be simulated based on the estimated π_i or determined first, and then the spray drift can be simulated from a normal or gamma according to the group.

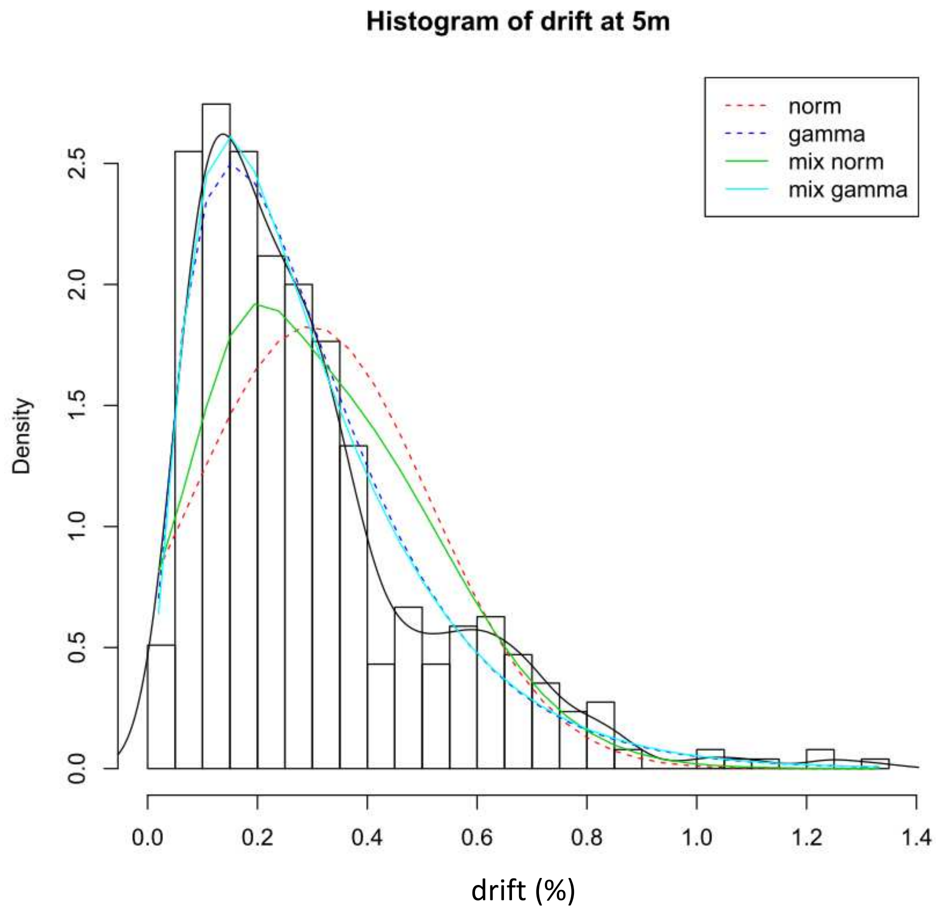


Figure 32: Comparison among the fitted normal, gamma, mixture of normal, and mixture of gamma for drift residue data at 5 m distance for arable. The mixture of normal and gamma has a stronger peak and heavier tail which agrees with the non-parametric probability density estimate.

Automated Trial Grouping

In contrast to the '*a priori*' approach, the goal of the 'automated trial grouping' was to determine trial groups by statistical means. A small number of groups was intended to be obtained. Variability of spray-drift deposition within the groups should be lower than between groups.

Different approaches were applied to 'automatically' determine trial groups and to assign the individual trials into them (*e.g.*, cluster Analysis, tree regression analysis).

In summary, statistical means to define trial groups did not result in robust, consistent and significant results (*e.g.*, trials were assigned to different groups for different distances). This can be attributed to the basically complex nature on how and to which extent the different parameters (*e.g.*, wind conditions, pressure) affected local spray-drift deposition. Therefore, automated grouping of trials by statistical means did not result in outcome that could reliably be used in landscape-scale ERA.

Mixed-Effect Model

In landscape-scale ERA, the PDFs developed herein will be sampled in order to estimate spray-drift deposition along an exposure path (swath) at a given distance (downwind) to the treated field. In doing so, care need to be taken on the question for which scale(s) independent samples can be drawn and for which scale(s) sampling needs to be regarded as being correlated.

Spatial scales occurring in a landscape-scale ERA are, *e.g.*, region (comprising a number of fields), the field (treated with a PPP and comprising a number of exposure paths), the exposure path representing a small swath (of about 1-10 m width) of spray-drift deposition downwind from a treated field, and finally the receptor, the discretised small part of a habitat, and therefore the smallest unit of analysis (Figure 31). The receptor represents the entity for which spray-drift deposition needs to be estimated.

Besides the trial (field-scale) with its specific conditions, a further important scale at which samples can be correlated is the exposure path (swath) along which spray-drift is leaving the field boundary and so leading to spray-drift deposits. As a tendency, spray-drift deposition along such a swath is either high or low the entire exposure path, *i.e.,* can be regarded as correlated.

Independent sampling for each receptor (*i.e.,* each distance from the field) based on the lumped analysis or the *a priori* grouping analysis suffers from the shortcoming that it may generate nonsensible results along an exposure path, such as a very low deposition at closer distances but a very high deposition at farther away distances. This problem can be solved by sampling the quantile first for an exposure path (swath) and then use this quantile of the fitted distributions at each distance as the sampled value. That way, the general trend over the distance is preserved and the variability among swaths is kept. However, the observed variability along the exposure path gets lost (corresponds to 100% correlation along the distances).

Instead of using the previously amended method using a pre-sampled quantile at exposure path-scale to avoid unrealistic sampling, an overall probabilistic distribution can be used for all the data at all distances and trials to account for the trend that the drift deposition decreases as the distance increases and keep both the in-swath and between-swath variability.

The Mixed-effect model is suitable for this purpose. A mixed model contains both fixed-effect parameters, as in the normal modelling procedure, plus random effects. The fixed-effects parameters represent the typical trend of the response and the independent variables, whilst the random effects component takes unit-to-unit variation into consideration so that the results can be generalised to the population level. In other words, it is a kind of hierarchical linear model with the assumption that the parameters related to each group come from an upper level distribution and the parameters that define this upper level distribution need to be estimated.

In the case of spray drift deposition, the trials can only represent a certain number of combinations of technological and environmental conditions like wind speed, nozzle type, pressure, *etc.* Different trials were considered as a categorical covariate representing "experimental units" in the deposition data set since the experimental conditions are similar for one trial but vary considerably across different trials. When the simulations are done, the trial conditions could be sampled from a population of conditions that are different from those of the observed trials (*i.e.,* the observed trials are regarded as a sample of this population). Therefore, the trial condition effect is not fixed but random. The observations in multiple swaths from each trial can be seen as repeated measurements. Here the variation of the deposition in each swath in one trial is assumed to come from the same function of distance plus some measurement error. The autocorrelation over distance and the correlation among the swaths are not considered.

As obtained in the lumped analysis section (above), the normal distribution parameters follow nicely a power curve over the distances. This leads to the model for hops defined by Equation 7.

Equation 7

$$
\begin{aligned}
&\log(\mathrm{Drift}_{ijk}) = \alpha_0 + \alpha_1 \log(\mathrm{Distance}_j) + \beta_{0k} + \beta_{1k} \cdot \mathrm{Distance}_j + \varepsilon_{ijk} \\
&i = 1,\ldots,n_k \quad j = 1,\ldots,8 \quad k = 1,\ldots,21 \\
&\alpha_0 \equiv \mathrm{Intercept} \quad \alpha_1 \equiv \mathrm{Distance\ Effect} \\
&\beta_{0k} \equiv \mathrm{Trial\ Effect\ for\ Trial}\ k \quad \beta_{1k} \equiv \mathrm{Distance\ Effect\ for\ Trial\ k} \\
&\beta_{0k} \sim \mathrm{NID}(0, \sigma_o^2) \quad \beta_{1k} \sim \mathrm{NID}(0, \sigma_d^2) \\
&\varepsilon_{ijk} \sim \mathrm{NID}(0, \sigma^2)
\end{aligned}
$$

It should be noted that this model can be expressed in different but equivalent forms. Essentially, there are 21 parallel regression lines (corresponding to the 21 trials). Drift deposition over distance in each trial varies around the base regression line in that trial. The parameters specific to each regression line come from an upper level distribution specified by the two normal with variances σ_0^2 and σ_d^2. The parameter estimates are obtained by restricted maximum likelihood (see Pinheiro & Bates 2000 for more details).

Software

Statistical analysis was done using the 'R' software package (version 2.12.2, CRAN 2011) and STATISTICA (version 8, Statsoft 2011). Data preparation was done using Microsoft Excel (version 2010).

5.3.5.4.4 Results and Discussion

In the following sub-sections, results and discussion of the different approaches are summarised, including recommendations on their potential use in landscape-scale ERA.

As the key results of the analysis are distribution (PDF) parameters and regressions over distances thereof, the full results were compiled in tables (csv-files) and transferred into an ORACLE database from which they can be accessed by landscape-scale models (*e.g.*, *Xplicit-Framework* exposure module*,* Section 5.3.4).

For each distribution 50th, 75th, 90th, 95th and 99th percentiles (quantiles) were calculated for the different distances (Section 5.3.5.4.3). The quantiles allow for an evaluation of the distributions, for comparison between the different distribution types and for comparison with official spray-drift deposition values ('Abdrifteckwerte', Rautmann *et al.* 2001).

Individual Trial Analysis

As described in Section 5.3.5.4.3, for each individual trial (of each crop type, by distance), five distribution types were fitted to the data: uniform, normal, lognormal, gamma, and beta.

In Table 9, an excerpt of the distribution parameters is shown.

In most of the cases, there are only 4-6 measurements, at most 10, for a given distance in each trial. With this small number of data points, there is no evidence to reject any type of distribution.

As the uniform distribution is the simplest among the distributions fitted and there is no evidence of any distribution to be preferred, the uniform distribution can be used to 'mimic' the variability observed in the individual trials in the landscape-scale model. However, there are drawbacks of not being able to sample drift depositions higher than the maximum observed ones or lower than the minimum observed ones. If the goals of a landscape-scale assessment include to assess also potential spray-drift depositions beyond the measured ones, the normal or gamma PDFs can be used, as these two types have the greatest popularity and as, especially the normal distribution, is commonly used as an approximation.

Table 9: Excerpt of the table on PDF parameters of the 'Individual Trial Analysis'

ID	Crop	PDF_Type	PDF_Param	Trial_ID	data_0m	data_1m	data_3m	data_5m	data_7.5m	data_10m	data_15m	data_20m	data_30m	data_50m
1	hops	norm	mean	24			9.31	3.65	0.88	0.54	0.14	0.09	0.06	0.04
2	hops	norm	mean	25			14.92	8.97	2.49	1.24	0.23	0.09	0.02	0.01
3	hops	norm	mean	26			14.38	6.99	3.21	2.13	0.66	0.31	0.13	0.01
4	hops	norm	mean	27			17.09	11.18	4.26	3.70	1.35	0.56	0.13	0.01
5	hops	norm	mean	28			7.87	7.17	4.92	3.86	1.96	1.01	0.31	0.05
6	hops	norm	mean	30			6.57	5.46	3.71	2.55	1.23	0.69	0.33	0.13
7	hops	norm	mean	31			6.71	6.06	3.99	2.82	1.29	0.68	0.16	0.05
8	hops	norm	mean	32			5.88	5.41	4.60	3.92	2.17	1.32	0.33	0.06
9	hops	norm	mean	33			8.17	6.41	3.90	2.81	1.12	0.42	0.08	0.01
10	hops	norm	mean	111						1.39		0.26		0.05
11	hops	norm	mean	113						3.80		1.74		0.07
12	hops	norm	mean	115			27.43	14.12	7.17	4.15	1.42	0.68	0.30	0.10
13	hops	norm	mean	116			10.19	2.73	0.63	0.17	0.06	0.07	0.01	0.01
14	hops	norm	mean	117			3.58	0.19	0.10	0.07	0.06	0.04	0.03	0.03
15	hops	norm	mean	118			16.47	10.15	6.04	3.42	1.46	0.73	0.21	0.09
16	hops	norm	mean	119			5.02	3.42	2.13	1.46	0.51	0.17	0.04	0.03
17	hops	norm	mean	120			14.14	10.86	8.51	7.37	3.90	1.54	0.65	0.20
18	hops	norm	mean	121			11.19	8.33	7.72	6.49	4.39	3.49	1.89	0.31
19	hops	norm	mean	122			11.97	6.22	3.40	2.46	0.71	0.32	0.12	0.07
20	hops	norm	mean	123			10.39	8.32	6.55	4.04	2.35	1.24	0.48	0.07
21	hops	norm	mean	124			7.90	5.89	3.64	2.76	2.35	1.60	0.30	0.06
22	hops	norm	sd	24			1.85	1.09	0.21	0.08	0.01	0.01	0.01	0.00
23	hops	norm	sd	25			3.42	2.25	1.19	0.48	0.03	0.02	0.00	0.01
24	hops	norm	sd	26			1.85	0.51	0.27	0.36	0.11	0.05	0.01	0.00
25	hops	norm	sd	27			2.84	1.51	0.19	0.40	0.13	0.12	0.01	0.00
26	hops	norm	sd	28			1.37	1.09	0.63	0.53	0.40	0.22	0.08	0.01
27	hops	norm	sd	30			0.74	0.58	0.49	0.18	0.12	0.12	0.03	0.03
28	hops	norm	sd	31			0.86	0.58	0.43	0.38	0.09	0.15	0.04	0.00
29	hops	norm	sd	32			1.17	1.14	0.92	1.04	0.67	0.42	0.09	0.01
30	hops	norm	sd	33			1.31	0.90	0.64	0.22	0.12	0.08	0.02	0.00
31	hops	norm	sd	111						0.70		0.15		0.02
32	hops	norm	sd	113						1.08		0.50		0.02
33	hops	norm	sd	115			8.03	6.55	2.78	1.27	0.32	0.06	0.05	0.02
34	hops	norm	sd	116			4.83	1.74	0.40	0.02	0.01	0.01	0.00	0.00
35	hops	norm	sd	117			2.18	0.16	0.01	0.01	0.01	0.01	0.00	0.05
36	hops	norm	sd	118			3.39	2.57	1.13	0.38	0.21	0.13	0.05	0.03
37	hops	norm	sd	119			0.95	0.58	0.25	0.14	0.06	0.03	0.01	0.01
38	hops	norm	sd	120			3.19	1.62	1.48	1.17	0.73	0.39	0.24	0.12
39	hops	norm	sd	121			6.70	4.30	3.96	2.58	0.30	0.74	0.37	0.07

Lumped Analysis

As described in Section 5.3.5.4.3, for each crop type all data at a certain distance were pooled, *i.e.,* PDFs were derived for each crop type and distance. Four distribution types were fitted to the data: normal, lognormal, gamma, and beta.

Resulting distribution parameters, exemplary graphs and statistics on comparison of goodness of fit between the distributions are summarised in Appendix 11.3.2 (Table A 5 to Table A 9, Figure A 1 to Figure A 21).

Regression analysis was performed for the PDF parameters of each distribution. The outcome allows to apply the PDFs also for distances between measured ones (interpolation).

The mean and standard deviation parameters from the normal fit agree well with simple fitted regression functions (Section 5.3.5.4.3). However, there are no obvious trends in the fitted parameters of other distributions over distance. So it is not clear how other distributions change over distance. It is generally expected that deposition should decrease as the distance increases, and thus the mean (and the standard deviation) parameters from normal decrease.

Table 10: Regression parameter (a,b) for normal distribution – lumped analysis.

Crop	Distribution parameter	Regression function	a	b	r^2
arable	mean	Equation 1	0.230	-0.983	0.984
arable	sd	Equation 1	0.027	-0.983	0.982
hops	mean	Equation 2	2.246	-0.105	0.965
hops	sd	Equation 2	1.755	-0.088	0.981
orchards-early	mean	Equation 2	2.437	-0.070	0.931
orchards-early	sd	Equation 2	1.770	-0.063	0.947
orchards-late	mean	Equation 1	3.936	-1.509	0.987
orchards-late	sd	Equation 1	3.258	-1.371	0.986
vines	mean	Equation 1	3.799	-1.974	0.926
vines	sd	Equation 1	2.905	-1.716	0.905

Pooling all trial data of a certain crop type into a single distribution (for a certain distance, 'Lumped-analysis') means that all variability inherited in these trials is represented by this PDF. Consequently, care needs to be taken when employing such PDFs in landscape-scale ERA: *e.g.*, in case that the pooled trials contain significant agricultural variability (*e.g.*, different types of spray-drift reducing nozzles), particular care should be taken when applying the PDFs at field-scale. However, such difficulties can become irrelevant when aggregating the results of a landscape-scale analysis at larger scales (*e.g.*, regional-scale). An alternative for better separation of trial conditions is offered with the '*a priori* grouping' analysis.

In most of the cases, the gamma fit seems to be acceptable according to Kolmogorov-Smirnov test. It has the smallest test-statistics of the Kolmogorov-Smirnov test and the smallest BIC values. The gamma distribution also has a moderately skewed profile (a stronger peak and a heavier tail), which agrees with what can often be seen in the observed deposition data. Therefore, when using lumped PDFs to represent variability of spray-drift depositions in landscape-scale approaches, there are statistical indications to prefer gamma without saying that other distributions cannot be used as well.

A priori Grouping of Trials

As described in Section 5.3.5.4.3, trials of each crop were grouped by trial conditions that most significantly affect spray-drift depositions ('Pressure', 'Wind-speed', 'Technology'). Definition of groups was done by expert judgement on the basis of frequency distribution of trial conditions ('*a priori* grouping'). For each *a priori* group, a normal and a gamma distribution was fitted to the trial data for each distance. The outcome of the '*a priori* grouping' approach can be used in landscape-scale ERA in two alternative ways:

i. **'TrialConditionGroup'**: A group is (randomly) selected according to the prevailing conditions. The PDF (normal or gamma) of the selected group represents variability of spray-drift deposition according to the group condition.
ii. **'Lumped-Analysis-2'**: A linear combination of the PDFs obtained for the individual groups (of a crop type) represents an improved 'lumped' analysis, *i.e.,* the total observed variability of spray-drift deposition (by distance).

The distribution parameters of the normal and gamma distribution fitted to the trial data of each *a priori* group for each distance, together with the coefficients of the linear combination, are summarised in Table 11.

As an example, the gamma distribution fitted to data of an orchards-late *a priori* group (group '1-1-2') for 3 m distance is shown in Equation 8 (using case 'i' above):

Equation 8:

$$deposition_{orchards\text{-}late\_3m\_group112} = \Gamma(3.5289, 0.4393)$$

$deposition_{orchards\text{-}late\_3m\_group112}$: spray-drift deposition (% of application rate) at 3 m of *a priori* group '1-1-2'

Γ(shape, rate): gamma distribution

The gamma distribution fitted to data of all orchards-late *a priori* groups for 3 m distance is shown in Equation 9 (using case 'ii' above):

Equation 9:

$$\begin{aligned} deposition_{orchards\text{-}late\_3m} = {} & 0.1923 \bullet \Gamma(3.5289, 0.4393) + 0.0659 \bullet \Gamma(9.8754, 1.1872) \\ & + 0.3297 \bullet \Gamma(6.0885, 0.9713) + 0.2418 \bullet \Gamma(2.3863, 0.3192) \\ & + 0.0989 \bullet \Gamma(6.7886, 0.4980) + 0.0220 \bullet \Gamma(13.1074, 2.2225) \\ & + 0.0495 \bullet \Gamma(8.5373, 0.6005) \end{aligned}$$

$deposition_{orchards\text{-}late\_3m}$: spray-drift deposition (% of application rate) at 3 m of all *a priori* groups

Γ(shape, rate): gamma distribution

An illustration of goodness-of-fit is shown in Figure 33.

Table 11: Example distribution parameters (normal, gamma) and linear combination coefficient (pi) for *a priori* groups (μ and *sd* are the mean and the standard deviation parameter of the normal, *shape* and *rate* are the parameters of the gamma distribution).

Crop	Distribution	Group	Distance	(µ, shape)	(sd, rate)	pi
arable	normal	1-1-1	1m	2.0565	1.6306	0.0571
arable	normal	1-1-2	1m	1.1815	0.8402	0.3429
arable	normal	1-1-4	1m	1.0137	0.7745	0.1714
arable	normal	1-2-1	1m	1.9530	2.0192	0.0286
arable	normal	1-2-2	1m	1.9861	1.1417	0.0857
arable	normal	2-2-2	1m	0.4339	0.2214	0.0857
arable	normal	2-2-3	1m	1.0881	1.0996	0.2286
arable	gamma	1-1-1	1m	1.2942	0.6293	0.0571
arable	gamma	1-1-2	1m	2.3826	2.0166	0.3429
arable	gamma	1-1-4	1m	1.7791	1.7551	0.1714
arable	gamma	1-2-1	1m	0.9961	0.5100	0.0286
arable	gamma	1-2-2	1m	3.2823	1.6526	0.0857
arable	gamma	2-2-2	1m	3.1559	7.2732	0.0857
arable	gamma	2-2-3	1m	1.9558	1.7974	0.2286
orchards-late	normal	1-1-2	3m	8.0340	4.5101	0.1923
orchards-late	normal	1-1-3	3m	8.3183	2.5112	0.0659
orchards-late	normal	1-2-1	3m	6.2685	2.7036	0.3297
orchards-late	normal	1-2-2	3m	7.4752	6.1514	0.2418
orchards-late	normal	2-1-2	3m	13.6322	5.1194	0.0989
orchards-late	normal	2-1-4	3m	5.8975	1.6737	0.0220
orchards-late	normal	2-2-2	3m	14.2178	4.6429	0.0495
orchards-late	gamma	1-1-2	3m	3.5289	0.4393	0.1923
orchards-late	gamma	1-1-3	3m	9.8754	1.1872	0.0659
orchards-late	gamma	1-2-1	3m	6.0885	0.9713	0.3297
orchards-late	gamma	1-2-2	3m	2.3863	0.3192	0.2418
orchards-late	gamma	2-1-2	3m	6.7886	0.4980	0.0989
orchards-late	gamma	2-1-4	3m	13.1074	2.2225	0.0220
orchards-late	gamma	2-2-2	3m	8.5373	0.6005	0.0495

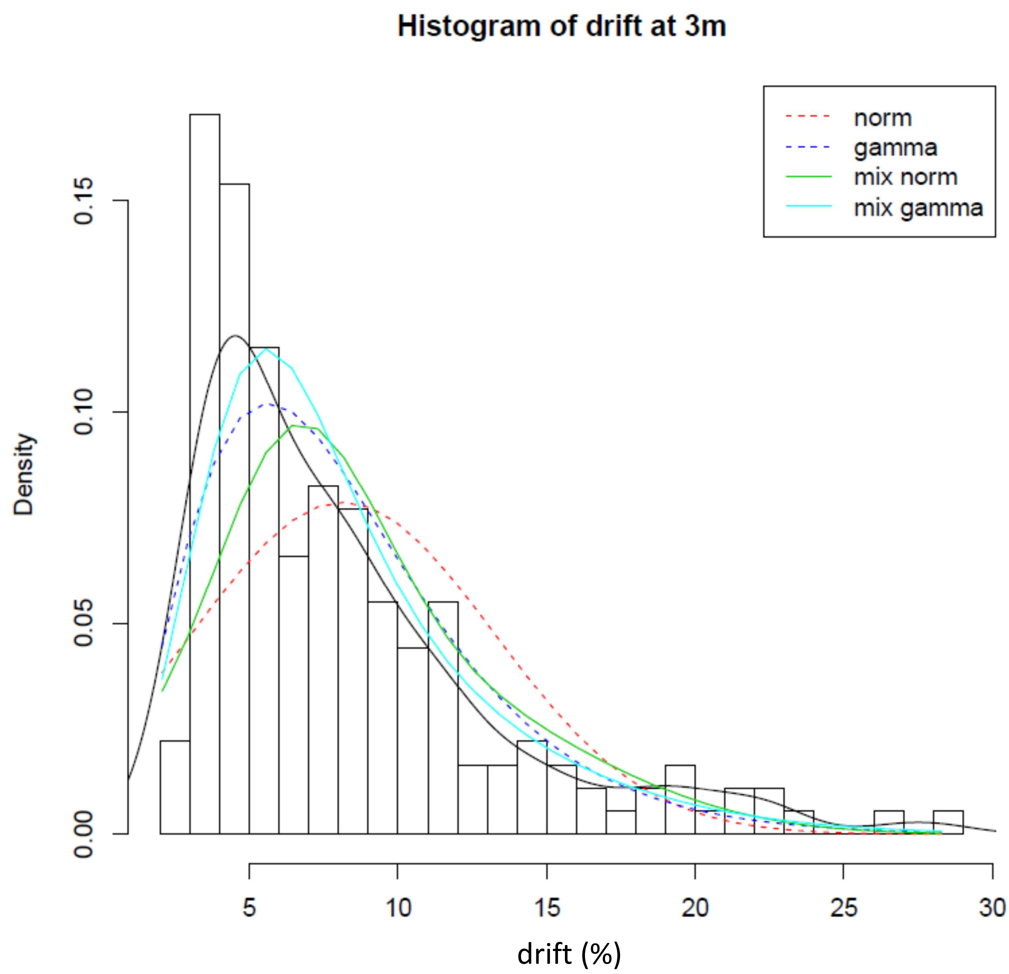


Figure 33: Frequency distribution of spray-drift depositions (bars) with non-parametric probability density estimate (black line), lumped PDFs (normal, gamma, dashed lines) and mixed PDFs (normal, gamma, solid lines) – orchards-late, 3 m distance.

As described in Section 5.3.5.4.3, previous analysis has shown that wind speed, spraying pressure and spraying technology (*e.g.*, nozzle and/or sprayer type) significantly affect spray-drift deposition in the vicinity of sprayed fields (which is in line with expert knowledge, *e.g.*, Rautmann pers. comm., 2010).

The range of conditions (wind speed, pressure, technology) prevailing during the measurements underlying the present analysis provided a reasonable basis for the grouping of trials. The number of groups was intended to be reasonably low in order not to try to be overly detailed and to keep an appropriate number of trails in each group for statistical analysis.

Distribution fitting was focused on using normal and gamma distributions: normal distributions were employed for the sake of statistical convention and to allow for comparison with already existing analyses (*e.g.*, Golla *et al.* 2011); gamma distributions were used as this distribution type had already shown its power in the 'Lumped-analysis' approach (above).

For each group of each crop, statistically significant distribution fits were obtained.

The resulting PDFs can be recommended to be used to represent variability of spray-drift deposition under the conditions prevailing in its '*a priori* group' (use case 'i' above), as well as to represent variability for the entirety of trials for each crop (use case 'ii', 'Lumped-Analysis-2', above). For the latter, the 'Lumped-Analysis-2' can be regarded as superior to the straightforward 'Lumped-analysis'. The same precautions should be taken into account when using variability obtained from the entire set of data of all trials of a crop type as described for the 'Lumped-analysis' (above).

Mixed-Effect Model

The Mixed-effect model is described in Section 5.3.5.4.3. The detailed results are provided in the report of Schad & Gao (2011, unpublished, please contact the author for details). Here, example results for hops are shown and the potential use of the results is described.

For hops, there are 870 observations in 21 different trials. The fitted regression lines are plotted in Figure 34 for each trial. In Table 12 are the parameter estimates and statistics associated with the fixed-effects terms, which defines the blue lines in Figure 34. Table 13 gives the trial-to-trial variance (standard deviation) for both the intercept and the slope parameter and the residual standard deviation. Table 14 shows the random effects added to the overall intercept and slope terms for each trial, which define the purple lines in Figure 34. These should be understood as the fixed effect observed in the field trials.

In terms of a Monte Carlo simulation (in landscape-scale approaches), two cases are considered:

1. In the first case, it is assumed that the simulated trial conditions are not known. A random effect need to be simulated first, as caused from the unknown variation due to the trial conditions, *i.e.*, generate $ß_{0k}$, $ß_{1k}$ according to normal distributions with mean 0 and standard deviation $\sigma_0 =$1.13 and $\sigma_d =$0.43, respectively. Also, the measurement error ε_{ijk} need to be generated following a normal distribution with standard deviation σ = 0.577. Then the $ß_{0k}$, $ß_{1k}$ and ε_{ijk} are replaced in Equation 7 with the simulated values. The $ß_{0k}$, $ß_{1k}$ represent the random part; their sampling randomly determines a trial, within which the measurement error ε_{ijk} has to be sampled for each exposure path (swath).
2. In the second case, suppose we can reproduce a similar condition as in trial number 24 (the trial conditions, and hence, the trial is randomly determined in a previous step in the land-scale approach). A $ß_{0k}$ = -0.65 and a $ß_{1k}$ = -0.12 can be used from Table 14 directly into Equation 7 and ε_{ijk} can be replaced with a simulated value according to a normal distribution with standard deviation σ = 0.577. Again, within the trial, sampling of the measurement error ε_{ijk} for each receptor on each exposure path (swath) represents the variability between them.

ε_{ijk} are sampled at receptor scale. Without ε_{ijk}, for a fixed ensemble of $ß_{0k}$ and $ß_{1k}$, the deposition follows the same fixed function of distance. From the modelling point of view, ε_{ijk} are measurement errors. From the sampling aspect, they are independent between receptor variability removing the distance factor.

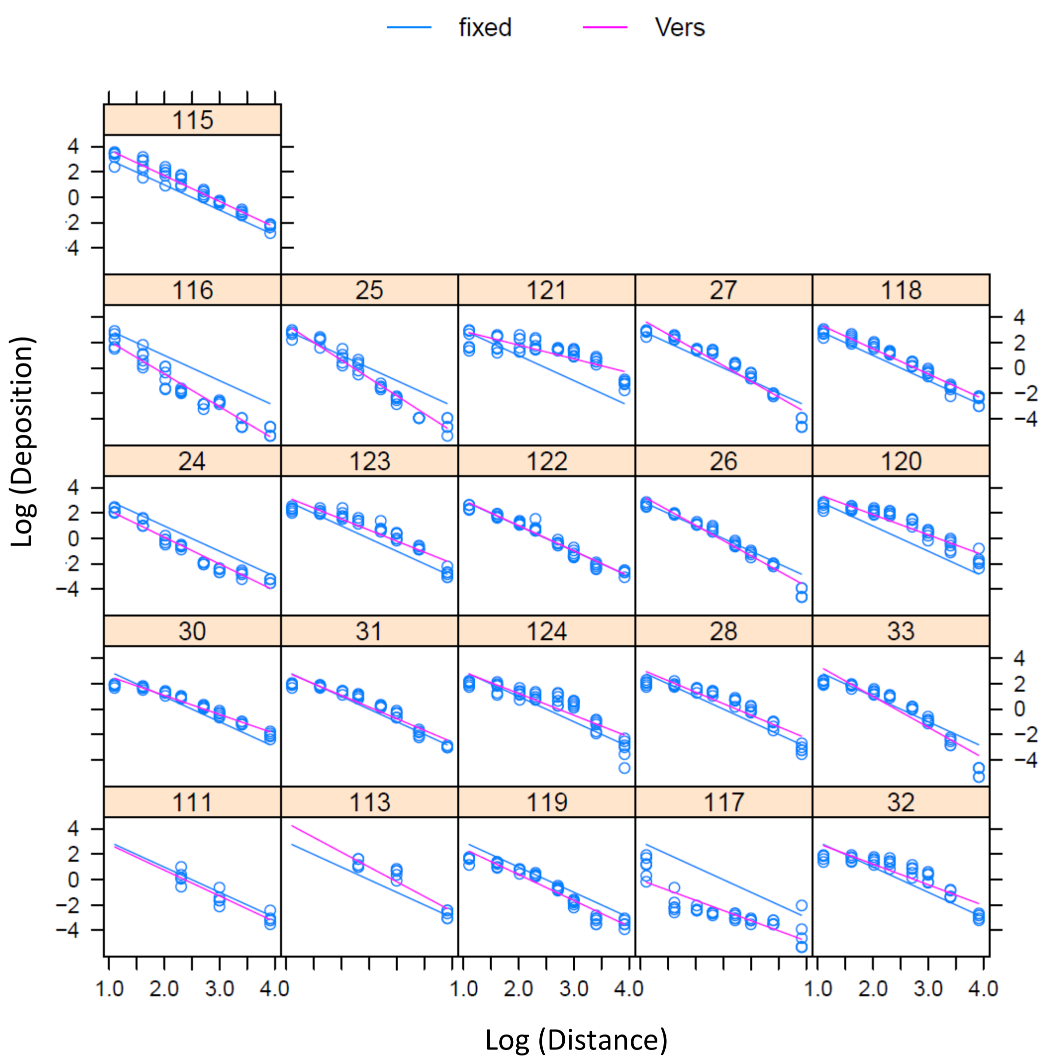


Figure 34: Mixed-effect model - illustration of fitted results for hops. The blue lines represent the overall trend of the drift deposition over distance. They are the same for all trials. The purple lines represent the different trends in each trial. These vary around the general trend, the blue line.

Table 12: Fixed Effects.

	Estimate	Std. Error	t value
(Intercept) α_0	4.9368	0.2563	19.26
log(dnum) α_1	-1.9810	0.0963	-20.57

Table 13: Random Effects.

Groups	**Name**	**Variance**	**Std.Dev.**	**Corr**
Trial	(Intercept) β_{0k}	1.2780	1.1305	
	log(dnum) β_{1k}	0.1819	0.4265	-0.653
Residual		0.3334	0.5774	

Table 14: Random Effects Estimates.

Trial	(Intercept) β_{0k}	log(dnum) β_{1k}
24	-0.65117	-0.11771
25	1.243802	-0.81221
26	0.864089	-0.41021
27	1.378414	-0.47948
28	-0.00643	0.173051
30	-0.87399	0.482327
31	-0.21816	0.152824
32	-0.48218	0.359235
33	0.900279	-0.44487
111	-0.14069	-0.04885
113	1.846234	-0.33762
115	0.809663	-0.04501
116	-0.26273	-0.5964
117	-3.39293	0.387851
118	0.510401	0.003322
119	-0.46923	-0.05858
120	0.123454	0.386815
121	-0.97602	0.895003
122	0.048524	-0.00806
123	0.053109	0.246119
124	-0.30444	0.272467

Due to complexity, neither the autocorrelation in one swath along the distance nor the correlation within one trial among swaths is considered in this modelling approach. Except for distance, other covariates were not included as predictors. Further work in this direction may improve the model.

This approach usually produces higher percentiles compared to previous approaches. One reason is that this model has two levels of variability which broadens the overall distribution. Moreover, the regression is done on the log of the observed values and the log of the distances, which can cause extremely large predictions of the deposition at small distances. However, this modelling approach shows a promising perspective for developing a comprehensive analysis framework by deriving an overall PDF and making scale-dependent predictions of future events based on that PDF.

Quantiles

Quantiles allow to evaluate the ranges of the distributions and for comparisons between them. The comparison of the 90th percentile predicted by the distributions (comprising all trials of a crop types, *e.g.*, 'Lumped analysis') with the official 'Abdrifteckwerte' is of particular interest with respect to the use of the distributions in regulatory ERA.

Detailed comparison between approaches and distributions are provided in the report of Schad & Gao (Bayer CropScience, 2011, unpublished, please contact author for details).

In Table 15 and Table 16, the 90th percentiles of the spray-drift depositions resulting from the different approaches ('Lumped-analysis', 'Lumped-analysis-2', 'Linear-Mixed-Effect Model') are compared to the 90th percentile values given in the official 'Abdrifteckwerte' (Rautmann *et al.* 2001). Differences of the 90th percentiles between the distributions and the 'Abdrifteckwerte' are presumably due to the fact that the latter are based on a non-parametric evaluation and due to the limited sampling number. The investigation of more systematic differences appear difficult due to comlex interactions of driving factors.

Table 15: 90th percentile spray-drift deposition (in % of application rate) of PDFs and official 'Abdrifteckwerte' by distance – arable.

		Distance [m]								
Crop	**Distribution**	**1**	**5**	**10**	**15**	**20**	**30**	**50**	**75**	**100**
arable	Abdrifteckwerte	2.77	0.57	0.29	0.20	0.15	0.10	0.06	0.04	0.03
arable	norm†	2.60	0.58	0.29	0.13	0.15	0.10	0.08	0.03	0.03
arable	lnorm†	2.45	0.59	0.32	0.13	0.16	0.11	0.10	0.03	0.02
arable	gamma†	2.45	0.57	0.29	0.12	0.15	0.10	0.08	0.03	0.03
arable	beta†	2.46	0.59	0.29	0.13	0.15	0.10	0.08	0.03	0.03
arable	norMix‡	2.57	0.59	0.29	0.12	0.15	0.10	0.08	0.03	0.03
arable	gammaMix‡	2.38	0.58	0.29	0.12	0.14	0.10	0.08	0.03	0.03
arable	log-LMEΔ	2.87	0.60	0.30	0.12	0.16	0.11	0.08	0.03	0.02
arable	logit-LMEΔ	2.83	0.61	0.30	0.12	0.16	0.11	0.08	0.03	0.02

† Quantiles resulting from 'Lumped-analysis'

‡ Quantiles resulting from 'a priori grouping – Lumped-analysis-2'

Δ Quantiles resulting from 'Linear-Mixed-Effect (LME) Model' ('logit' uses 'log(drift/(1-drift))' in Equation 7)

Table 16: 90th percentile spray-drift deposition (in % of application rate) of PDFs and official 'Abdrifteckwerte' by distance – high crops.

		Distance [m]						
Crop	**Distribution**	**3**	**5**	**10**	**15**	**20**	**30**	**50**
hops	Abdrifteckwerte	19.33	11.57	5.77	3.84	1.79	0.56	0.13
hops	norm†	19.88	12.32	5.72	3.23	2.03	0.92	0.18
hops	lnorm†	19.54	12.32	6.23	3.72	2.16	0.76	0.18
hops	gamma†	19.50	12.20	5.83	3.33	1.99	0.78	0.17
hops	beta†	19.65	12.23	5.83	3.33	1.99	0.90	0.18
hops	norMix‡	19.25	12.12	5.80	3.44	2.11	1.01	0.19
hops	gammaMix‡	19.49	12.41	5.88	3.49	2.04	0.81	0.16
hops	log-LMEΔ	NA	16.13	4.87	2.37	1.47	0.77	0.32
hops	logit-LMEΔ	NA	15.07	4.93	2.40	1.49	0.77	0.31
orchards-late	Abdrifteckwerte	15.73	8.41	3.60	1.81	1.09	0.54	0.22
orchards-late	norm†	14.66	8.08	3.50	1.89	1.09	0.51	NA
orchards-late	lnorm†	14.11	8.52	4.75	2.70	1.40	0.59	NA
orchards-late	gamma†	14.22	8.17	3.81	2.06	1.16	0.52	NA
orchards-late	beta†	14.32	8.17	3.80	2.05	1.11	0.52	NA
orchards-late	norMix‡	14.98	8.26	3.53	1.96	1.10	0.54	NA
orchards-late	gammaMix‡	14.55	8.40	3.54	1.99	1.10	0.52	NA
orchards-late	log-LMEΔ	21.39	9.10	3.11	1.74	1.18	0.69	NA
orchards-late	logit-LMEΔ	19.44	8.98	3.14	1.75	1.18	0.68	NA
orchards-early	Abdrifteckwerte	29.20	19.89	10.89	5.93	3.51	1.71	0.25
orchards-early	norm†	26.54	25.01	12.94	6.67	4.53	2.48	0.32
orchards-early	lnorm†	29.90	26.11	11.47	6.08	3.82	1.87	0.26
orchards-early	gamma†	27.94	24.75	11.42	6.08	3.81	1.86	0.25
orchards-early	beta†	27.57	25.04	11.00	6.03	3.54	1.74	0.26
orchards-early	norMix‡	26.72	25.41	11.02	5.86	3.60	1.79	0.27
orchards-early	gammaMix‡	27.23	24.05	15.70	7.95	5.06	2.81	0.44
orchards-early	log-LMEΔ	84.78	57.25	15.03	7.88	5.00	2.72	0.43
orchards-early	logit-LMEΔ	50.43	40.69	10.89	5.93	3.51	1.71	0.25
vines	Abdrifteckwerte	8.02	3.62	1.23	0.65	0.42	0.22	0.10
vines	norm†	6.30	3.53	1.23	0.58	0.31	0.04	0.08
vines	lnorm†	7.21	4.07	1.48	0.63	0.33	0.03	0.07
vines	gamma†	6.67	3.69	1.29	0.59	0.31	0.04	0.07
vines	beta†	6.65	3.68	1.26	0.59	0.31	0.04	0.08
vines	norMix‡	6.34	3.61	1.26	0.59	0.31	0.04	0.08
vines	gammaMix‡	6.54	3.59	1.27	0.58	0.31	0.04	0.08
vines	log-LMEΔ	16.10	5.20	1.22	0.55	0.32	0.08	0.04
vines	logit-LMEΔ	14.45	5.08	1.22	0.55	0.32	0.08	0.04

† Quantiles resulting from 'Lumped-analysis'; ‡ Quantiles resulting from 'a priori grouping – Lumped-analysis-2'; Δ Quantiles resulting from 'Linear-Mixed-Effect (LME) Model' ('logit' uses 'log(drift/(1-drift))' in Equation 7)

Conclusions

Exposure (and risk) of Non-Target-Organisms due to spray-drift depositions of PPPs into their habitats depends on environmental and agricultural conditions during PPP spraying. These conditions can vary significantly. With the objective to provide more realistic risk estimates, landscape-scale ERAs need to take such variability into account.

Currently available empirical data on spray-drift deposition were generated with the aim to provide a basis for Tier-1 ERA for spray-drift ('standard scenario', Rautmann *et al.* 2001). Consequently, measurement conditions were intentionally focused on conservative conditions (*e.g.,* comparably high wind speeds) that might reasonably occur in the range of good agricultural practice, and hence, the use of PDFs based thereof inherently introduces a conservative momentum to landscape-scale ERA.

Using the same data as underlying the official 'Abdrifteckwerte' (Rautmann *et al.* 2001), the PDFs derived herein represent the variability inherent to the official measurements. As such, especially the 90th percentiles of the PDFs (P90) were calculated and compared to the official 'Abdrifteckwerte'. P90 of the PDFs were close to the officially reported values in the 'Abdrifteckwerte' (some slightly lower, some slightly higher, which can be due to the calculation procedure used to generate the 'Abdrifteckwerte', Rautmann *et al.* 2001). This is regarded as an appropriate result for the use of the PDFs in regulatory ERA. Moreover, consistently lower P90 obtained in distribution fitting can help to reconsider the calculation procedure of P90 spray-drift depositions in future measurement campaigns with respect to the intended protection goal.

In summary, empirical models (PDFs) were developed that allow to represent variability of spray-drift deposition as underlying the official 'Abdrifteckwerte', adequate for landscape-scale risk characterisation. The results offer the study director of a landscape-scale approach some degrees of freedom to use different empirical models, *e.g.*, depending on the scale at which spray-drift variability is to be represented or the scale of the aggregation of the outcome of a landscape-scale risk characterisation (*e.g.*, local or regional).

Recommendations for the use of PDFs

There are different ways to make use of the analysis:

i. Sampling based on the individual trial analysis:

For individual trial based sampling, it is the user's choice which type of distributions to use since there is no obvious evidence to prefer one distribution over another. With a small sample size, *e.g.,* 4, the estimation of the mean or the standard deviation is also questionable. The uniform distribution is recommended to be used, so that the samples will cover a range of possible values instead of concentrating in the range of the peak value of the estimated distribution, which is questionable because of the small sample size.

ii. Sampling based on lumped analysis:

Based on the Bayes Information Criterion (BIC) and the Kolmogorov-Smirnov (KS) tests, the results indicate that the gamma distribution is overall better suited than the other three distributions. Thus, the gamma distribution is recommended as the best fit distribution.

It may generate nonsensible results such a low deposition at near distances but a much higher deposition at farther distances if sampled independently for each distance (*i.e.,* ignoring potential correlation in spray-drift deposition along an exposure path (swath). This problem can be fixed by sampling the quantile first and then use the same quantile for all distances of an exposure path. However, this could reduce variability in the data over distances. Analysis of less strict correlation between distances in the same exposure path needs further work.

iii. Sampling based on *a priori* grouping analysis:

Since 'automated grouping' of trials did not provide consistent results over distance, clustering over all distances directly based on the numerical values is not reliable and hard to explain. Therefore, the use of the *a priori* grouping analysis results is recommended for simulation.

The outcome of the '*a priori* grouping' approach can be used in landscape-scale ERA in two alternative ways:

i. **'TrialConditionGroup'**: A group is (randomly) selected according to the prevailing conditions. The PDF (normal or gamma) of the selected group represents variability of spray-drift deposition according to the group condition.
ii. **'Lumped-Analysis-2'**: A linear combination of the PDFs obtained for the individual groups (of a crop type) represents an improved 'lumped' analysis, *i.e.,* the total observed variability of spray-drift deposition (by distance).

Outlook

Ideally, in landscape-scale ERA, spray-drift modelling should allow to estimate local spray-drift deposition in dependence of local weather and agricultural conditions that can prevail in the relevant spatiotemporal domain. This is required not only as deposition on two-dimensional (2d) ground level but also on more complex 3d natural structures (*e.g.*, vegetation).

Currently, developments of mechanistic spray-drift models are ongoing (*e.g.*, Holterman *et al.* 1997, Miller & Hadfield 1989, Endalewa *et al.* 2010). In the future, such models are expected to be capable of estimating spray-drift deposition in dependence of most significant spraying conditions (weather and agricultural).

At present, variability in spray-drift deposition can be represented by the variability observed in the available spray-drift measurements. Such empirical models represent weather and agricultural as prevailing during the measurements. So far, the objective of the measurements has been to focus on conservative conditions in order to derive spray-drift deposition data for lower-tier RA. However, assuming such conditions to occur everywhere and all the time can be regarded as overly conservative for landscape-scale RA. Thus, the distribution of spraying conditions needs to be taken into account (*e.g.*, spray-drift measurements for low wind speeds, which could also show spray-drift towards all directions around a sprayed field and not only in a single downwind direction).

Therefore, future spray-drift measurement campaigns should consider the use of the data in landscape-scale and mechanistic spray-drift exposure modelling.

5.3.5.5 Modelling Exposure Due to Spray-drift – Spray-drift Filtering by Riparian Vegetation

This section provides an executive summary of a literature evaluation on spray-drift filtering by riparian zone vegetation ("*Spray-Drift Filtering by Riparian Zone Vegetation in Spatially Explicit Aquatic Exposure Assessment - A Literature Evaluation*", (Schad T, Ohliger R, Schulz R, 2009, Bayer CropScience, unpublished). In this literature evaluation, empirical filter effects were transferred into PMFs which represent the variability of spray-drift filtering for certain PPP application methods, riparian vegetation types and conditions.

The *Xplicit-Framework* is designed to assign such models in its exposure module, and so, to apply the represented variability at user-defined scales in the exposure assessment. The spray-drift filter model can be employed with any other exposure models defined by the user (*e.g.*, Section 5.3.5.4).

Spray-drift depositions of PPPs into small water bodies (WBs) occurring in field vicinity are a major concern in aquatic RAs. Standard aquatic RA scenarios ('lower-Tier') do not assume any barrier between the field and the WB. However, if a WB is not completely artificial (*e.g.*, concrete canal), it often is naturally accompanied by riparian vegetation. For natural WBs, not only herbaceous vegetation is typically present, often high perennial vegetation (bushes, trees) occurs as well. All three vegetation layers (herbaceous, bushes, trees) potentially filter spray-drift, whereby high perennial is of particular effectiveness.

Taking the process of spray-drift filtering into account can significantly improve the characterisation of aquatic risk in spatially explicit RA, *e.g.*, using the Xplicit approach (Section 5.3, Schad & Schulz 2011). The basic problem is how to adapt measured filter effects to available geodata, with particular consideration of scale dependencies of variability, while maintaining a required certainty level in the RA. On the one hand, filter data gathered from literature does not represent systematic experiments that were designed for the present purpose and, on the other hand, riparian vegetation is typically represented by geodata in only simple land cover categories. Therefore, a robust and reasonably conservative approach was proposed using straightforward categorisation of (i) the vegetation type in the filter experiments, (ii) the measured filter efficacy, and (iii) the riparian vegetation represented in geodata used in landscape-scale RA:

- The measured filter effect was assigned to predefined categories adopted from spray-drift reducing technology (25%, 50%, 75%, 90%, *e.g.*, FOCUS 2007a, 2007b).
- Two filter vegetation types, *low* and *high*, were defined, corresponding to grass/herbaceous or bushes/trees (perennial).
- Temporal variability of vegetation density was accounted for by using two leaf development stages ('*leaves*', '*no leaves*'). Long-term temporal variability (*e.g.*, due to vegetation growth, decay, maintenance) has to be considered in the representation of riparian vegetation in geodata.
- Two different crop types were considered, typically related to different spraying technologies: *arable* (boom sprayer) and *high* (axial sprayer, *e.g.*, orchards, hops, vines).
- All variability that occurs below the scale of the filter vegetation as such, *i.e.*, within the vegetation (*e.g.*, porosity) or within the scale of the local experimental set-up (*e.g.*, wind

speeds, further agricultural conditions: *e.g.*, nozzle, pressure, driving speed) was implicitly transferred as conditions present when applying the filter effect in landscape-scale ERA.

- Filter efficacy was presented as conservative deterministic and as PMFs (Probability Mass Functions).

Two cases illustrate the proposed use in landscape-scale ERA:

1. **Local scale data (high resolution)**: Geodata is available in a resolution and quality that allows characterisation of vegetation at a local scale (≈10^0-10^1 m): *e.g.*, high-resolution remote sensing imagery allow to locally distinguish between bare, grass/herbaceous, bushes/trees. Deterministic or PMF filter efficacy data can be assigned to a local vegetation object of a certain type (*e.g.*, group of bushes) present in the geodata. Local vegetation conditions (*e.g.*, density) could be verified by ground truthing, if applicable. Minimum vegetation width thresholds could be used in local exposure calculation. Variability represented in a PMF is sampled at local scale, *i.e.*, for each exposure path reaching from a field edge point to a WB segment. Assessments on the spatial variability of exposure and risk can be made at local scale (*e.g.*, probability of a trigger value to be exceeded for >10% for each individual WB segment).
2. **Higher scale data (medium resolution)**: Geodata provides information on frequencies of the occurrence of riparian vegetation at scales beyond local (≈10^2-10^4 m, *e.g.*, LUA 2005, 'Gewässerstrukturgütekartierung' in Germany characterising WB segments of 100-1000 m length by vegetation type). For exposure paths at local scale, first the corresponding PMFs on the *occurrence* of a vegetation type is sampled, then, second, a filter efficacy is applied as in (1), using a deterministic or PMF filter effect). Consequently, risk characterisation has to be restricted to the smallest scales at which vegetation data is provided (*e.g.*, WB segment or regional), *i.e.*, an assessment for an individual local WB segment cannot be made.

The review was done in 2008 and started with already available reviews (*e.g.,* FOCUS 2007a, 2007b, Mackay *et al.* 2002), consulted >30 publications relevant for conditions in European landscapes (*e.g.*, Hewitt 2001, Ucar & Hall 2001, van de Zande *et al.* 2000a-c, 2004) and was supported by personal communication (*e.g.*,. van de Zande (IMAG-DLO), H Koch (DLR), R Friesleben (BCS), A Chapple (BCS), B Golla (JKI)). In total, 59 filter values were considered. The review is not regarded exhaustive. Spray-drift interception by emerged water plants (*e.g.*, Dabrowski *et al.* 2005) which can further reduce deposition or at least cause a temporal stretching, hence, peak concentration reduction (with potential subsequent wash-off) was not taken into account. Also, geometric effects on spray-drift deposition due to the fact that the water level of a WB is typically below ground level were not investigated.

Some authors reported filter effect *ranges* instead of individual values. In this case, the minimum and maximum values reported were assigned to the predefined categories.

Table 17 summarises statistics on the compiled filter efficacies by filter vegetation category. The majority of experiments were conducted with *high* vegetation (*e.g.*, bushes, hedges, trees) in '*leaves*' (vegetated) development status, for which a median filter efficacy of 86% was obtained. For the same vegetation type in '*no leaves*' development status, a median of 45% filter effect was found. For *low* filter vegetation in vegetated development status, a median filter efficacy of 67% was obtained.

Table 17: Number of observations (n) and filter efficacy ([%], Px: x^{th} percentile) for different vegetation types and development stages.

Vegetation	n	Mean	Median	Min	Max	P10	P25	P75	P90
high, leaves	39	84.2	**86.0**	63.0	99.5	70.0	75.0	92.0	97.0
high, no leaves	10	43.9	**45.0**	10.0	80.0	12.5	20.0	68.0	79.5
low, vegetated	10	67.0	**67.0**	42.0	90.0	47.0	55.0	77.0	87.5

The theoretically eight different cases resulting from the combination of filter vegetation type, vegetation development status and crop type reduced to three essential cases: filter effects of *high* vegetation were pooled for both application types (*high* and *low* crops) and for *low* filter vegetation, only applications in *low* crops and in *leaves* (*vegetated*) development status were investigated.

Table 18 summarises the proposed deterministic spray-drift filter efficacies considered reasonably conservative following the data in Table 17 and the frequency distributions shown in Figure 35 to Figure 37.

Table 18: Deterministic spray-drift filter efficacy proposed for different riparian vegetation types, crop types and riparian vegetation development stages ('*leaves*', '*no leaves*').

Vegetation Type	Crop Type	Leaves	No Leaves
high, hedges, bushes, trees	*high* or *low*	75%	25%
low, grass/herbaceous	*low*	50%	(25%)†

† Estimated proposal for status of considerable natural remains of grass/herbaceous riparian vegetation during winter period; not cut or mulched (otherwise 0% has to be assumed).

Categorised filter efficacy obtained for *high* vegetation in '*leaves*' development status is shown in Figure 35. 44% of the observed filter efficacies were found to be >90%, and 80% to be ≥75%. The minimum efficacy was found to be 63% (Table 17) which is close to the proposed deterministic value of 75% (Table 18). In comparison, in the Dutch authorisation process of PPPs, the assessment scheme for spray-drift entries into WBs considers spray-drift reduction rates of 90% for windbreaks at full leaf (Wenneker 2005). A 90% filter effect can be justified in case of particular local conditions, *e.g.*, dense windbreak hedge or natural vegetation of all three vegetation layers present (herbaceous, bushes, trees). In case local geodata provides indications for considerable vegetation porosity (*e.g.*, gallery of poplar trees with gaps, without bushes underneath and cut grass surface) lower filter effects can be more appropriate (*e.g.*, 50%).

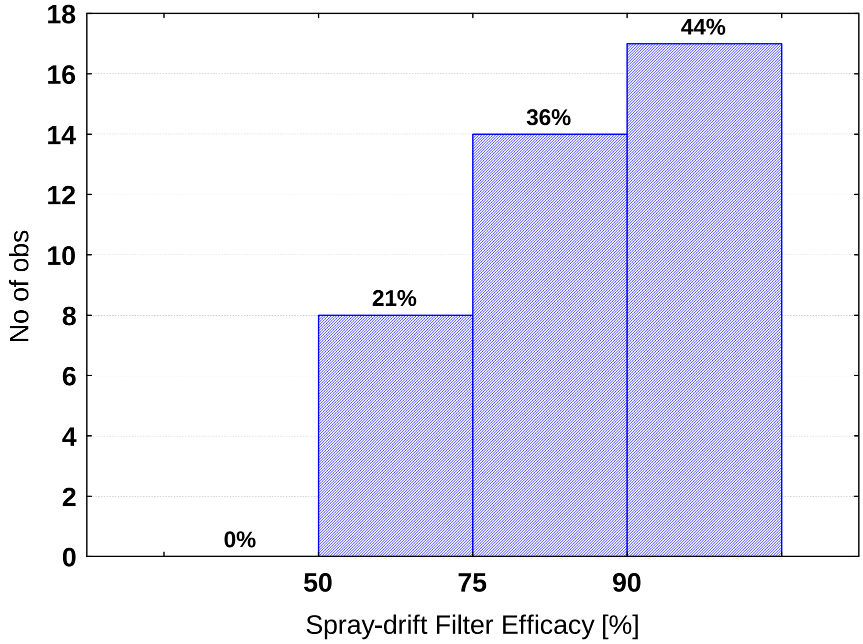


Figure 35: Filter efficacies of *high* vegetation in '*leaves*' development status.

Data for *high* vegetation in '*no leaves*' status is shown in Figure 36. As the graph shows, 60% of the measurements are above the proposed deterministic filter efficacy of 25%, 40% are below. A median of 45% filter efficacy was obtained (Table 17). In comparison, given a certain constitution of a windbreak, the Dutch authorisation considers 70% filter efficacy at early vegetation development stages (Wenneker 2005).

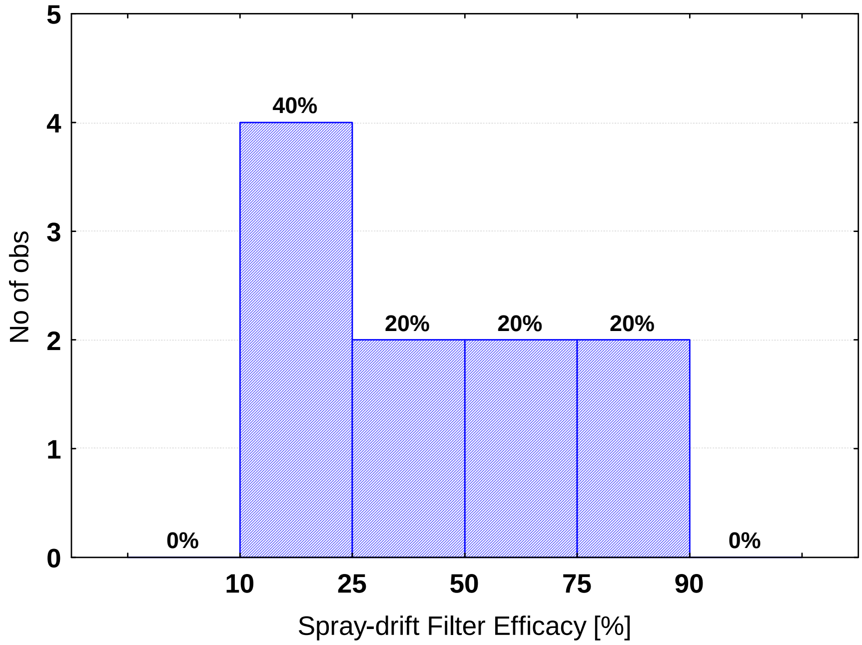


Figure 36: Filter efficacies of *high* vegetation in '*no leaves*' development status.

Natural streams and ecologically particularly viable ditches are typically accompanied by herbaceous riparian vegetation and, hence, the spray-drift filter potential of this vegetation apparently affects aquatic RA on landscape-scale.

The spray-drift filter efficacy of grass/herbaceous vegetation was studied for applications in *low* crops. For filter vegetation around 0.5 m to >1 m height (*e.g.*, tall grass/flower mixture), which can be regarded as typical for a natural riparian zone in vegetated status ('*leaves*'), a 50% spray-drift filter efficacy was proposed as a reasonably conservative deterministic value (Table 18). As shown in Figure 37, 90% of the measurements are ≥50%. These results apply when WB banks are not in a temporarily maintained status due to cutting or mulching.

When ditches and stream banks are not cut during or immediately before the non-vegetated period (winter) the remains of this grass/herbaceous vegetation built a three-dimensional structure of considerable height and density with a corresponding potential to filter spray-drift. Quantitative data addressing the filter efficacy at that status could not be obtained. However, comparing the structure of grass/herbaceous remains with the experimental set-up of the studies, the filter efficacy might be lower than that during the vegetated status, yet, likely >0%. Therefore, a deterministic 25% efficacy is preliminary proposed for these conditions (Table 18).

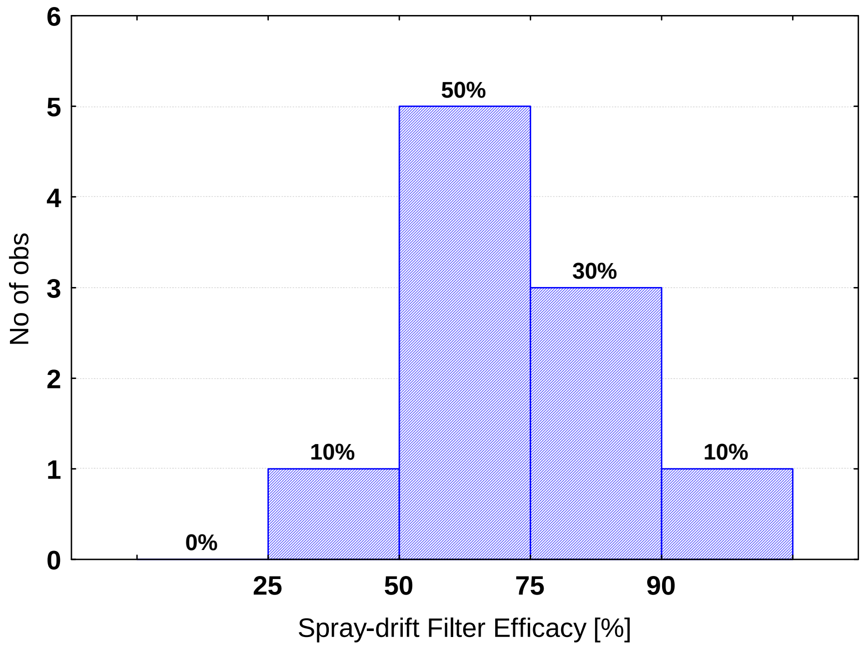


Figure 37: Filter efficacies of *low* vegetation in '*leaves*' (vegetated) development status.

There is agreement in the data and reports that windbreaks provide good protection immediately in the lee. Increase of depositions at larger distances behind the windbreak do not apply to the intended use of the filter values for aquatic risk characterisation of comparably small WBs, as the water surface is typically located in the shelter zone of the riparian vegetation. For larger streams and rivers, spray-drift filtering can be of less importance with respect to reduce risk, due to their large water surface area, large water volume and typically larger distance to crop.

Spray-drift reducing factors, either naturally present or agricultural ones, can be combined to overall reductions as long as they are independent of each other. This presumably applies largely to the use of drift-reducing technology (*e.g.*, low drift nozzles) and the occurrence of drift filtering vegetation. In this case, factors combine to an overall reduction. As filter effect of *high* vegetation is assumed to already include filter efficacy of grass/herbaceous, these factors should obviously not be combined.

For the purpose of quantifying the variability of spray-drift filtering of riparian vegetation in spatiotemporally explicit and probabilistic ERA, more adapted and systematic measurements could be considered in the future. Also, data could be fitted to continuous PDFs (*e.g.*, lognormal, gamma). Besides mitigation by riparian vegetation filtering, further naturally present factors could be considered, *e.g.*, filtering of emerged water plants (Dabrowski et al 2005) or effects due to WB geometry and water surface level. Both factors would require to address the environmental fate of the filtered amounts of PPP (*e.g.*, photo-degradation, wash-off).

5.3.5.6 Recolonisation Potential of Habitat Segments - *Xplicit-Distance*

Accepting effects of PPPs to Non-Target-Organisms is related to effects' transitional characteristics (*e.g.*, SPGs, Section 4.3.2.1) often discussed in terms of population *recovery* back to a certain status ('control'). In simple terms, recovery can happen from within a population (or habitat) and/or due to exchange with external populations (or habitats), hence, due to *recolonisation*. The processes that contribute to and drive recolonisation and the ecological conditions can be diverse; major factors are, *e.g.*, dissipation (and bioavailability) of the substance that caused the effect and species dispersal potential.

Recolonisation can hardly be explicitly modelled when not a specific species is in focus of the RA, but effect characterisation represents a higher-level taxonomic group of Non-Target-Organisms, *e.g.*, NTAs, (due to deputisation principle at lower-Tier), or in absence of species related recolonisation models. In this situation, the risk characterisation can be improved by estimating the recolonisation potential of 'affected' habitats (or habitat segments). This can be done by calculating distances an organism would have to travel from unaffected to affected habitats (segments). These distances can be calculated in spatial and temporal scales (*e.g.*, "*how long would it take until the substance has dissipated to no-effect-levels and so, the habitat could be recolonised?*").

An evaluation module was developed (in cooperation with R Vamshi and C Holmes, Waterborne-Environmental Inc.) capable to respond (spatial) recolonisation distances from essentially two inputs: geodata on the land use/cover and *Receptor* data representing affected/unaffected habitat sections. The module is designated '*Xplicit-Distance*' and splits in two parts:

i. An ArcGIS Server geoprocessing service (*XDist*) which accepts *Receptors* of RA endpoint (*e.g.*, TER) violation and returns for each of these the (shortest) distance to an un-affected habitat location.
ii. A web-service (*XCommunicate*) to access the geoprocessing part and for data exchange.

The module has been utilised via the *Xplicit-Assess* component (*XA*, Section 5.3.4.4), for post-processing and evaluation of the outcome of Xplicit simulations. *Xplicit-Distance* was employed in landscape-scale risk characterisation for Non-Target-Arthropods (case study, Section 6.1). The web-service was successfully implemented and ran at Waterborne (Waterborne 2010) and BCS servers. The module can also be employed via *Xplicit-Processors* as an *Associated*-(effect-)*Model* (Section 5.3.4.10).

The following items briefly characterise the use of the *Xplicit-Distance* module via *XA*:

- *XA* sends a list of 'affected' *Receptors* and receives the return data with the (shortest) distances to 'un-affected' habitats (segments).
- The *Xplicit-Distance* geoprocessing service resides on an ArcGIS server (*e.g.*, at BCS or Waterborne, *i.e.*, from BCS perspective 'on premisis' or 'off-premisis').
- The *Xplicit-Distance* geoprocessing model (*XDist*) is published as a "tool layer".
- The data to be stored and processed are in ESRI vector point format; vector-based operations (*e.g.*, *Near* or *GenerateNearTable* geoprocessing) are used.

- The list of 'affected' *Receptors* can have upwards of 1,000,000 *Receptors* (numeric ID of *Receptors* are provided). Each Xplicit (Monte Carlo) simulation generates one list.
- The *Xplicit-Distance* geoprocessing service 'knows' the full landscape (uploaded before the actual use of the service) and reads a list of Xplicit *MC run* results. *Xplicit-Distance* processes each run and compiles the output table containing the (shortest) distance to the 'un-affected' *Receptor* and the associated *Receptor* ID. The geoprocess is initiated by *XA* via *XCommunicate* and contains the following process steps:
  1) Receive data from *XCommunicate* (or user when running in interactive mode).
  2) Parse data for each run.
  3) Call *XDist* geoprocessing service for each run.
     a. Create a layer of only IDs for 'affected' (Input Features).
     b. Create a layer of only IDs for 'un-affected' (Near Features).
     c. Compute the distance of each Input Feature to the nearest Near Feature using the Near of GenerateNearTable geoprocessing tool (cost-path considered for subsequent version).
  4) Return data with original ID, distance to closest 'un-affected' *Receptor*, and *Receptor* ID.
- *XDist* is a GIS service that is called for each individual MC run. Results are compiled and analysed in *XA*.
- *XDist* uses the ArcGIS ModelBuilder. In Interactive mode (from within ArcMap or ArcCatalog) the dialog that opens will ask for three input parameters: Input Landscape (Shapefile or Geodatabase feature class), File containing the 'affected' *Receptor* IDs (Text file), Name of the output file (Text file).
- *XCommunicate* sends the list of 'affected' *Receptors* and receives a return table with the (shortest) distance to 'un-affected' *Receptors*, processed by *XDist* (Figure 38).
- *XCommunicate* publishes three web methods: GetDataFromWebserver(), GetTicketStatus(), SendDataToWebserver(). Example Use Case (main steps):
  1) Initiation of the web service class; configuration in XML file.
  2) *XA* (Client) calls the Web service class using the exposed <Web method>, passing the input data (ReceptorID's); if data is beyond a pre-set size limit then split.
  3) Upload summary and all data to Web server.
  4) Web server receives input data, generates ticket with summary of input data and time stamp.
  5) Client receives and stores ticket as a state variable of the class.
  6) Periodically client uses ticket to check GIS process status; if GIS process status on Web server is 'Complete', then Client downloads GIS results data, *e.g.,* <ReceptorID>,<RecolonizationID>,<Distance> from the Web server and finishes process.
- Initially, calls from *XA* to *Xplicit-Distance* are synchronous, *i.e.,* the *XA* evaluation process waits for response. Initially, only one project is executing at a time via *XA*.

- Implementation: Microsoft .NET Framework (Microsoft 2012b), ArcGIS, ArcGIS Server Enterprise (Esri 2012).
- Web-service: IIS installed on a Web Server machine and running.

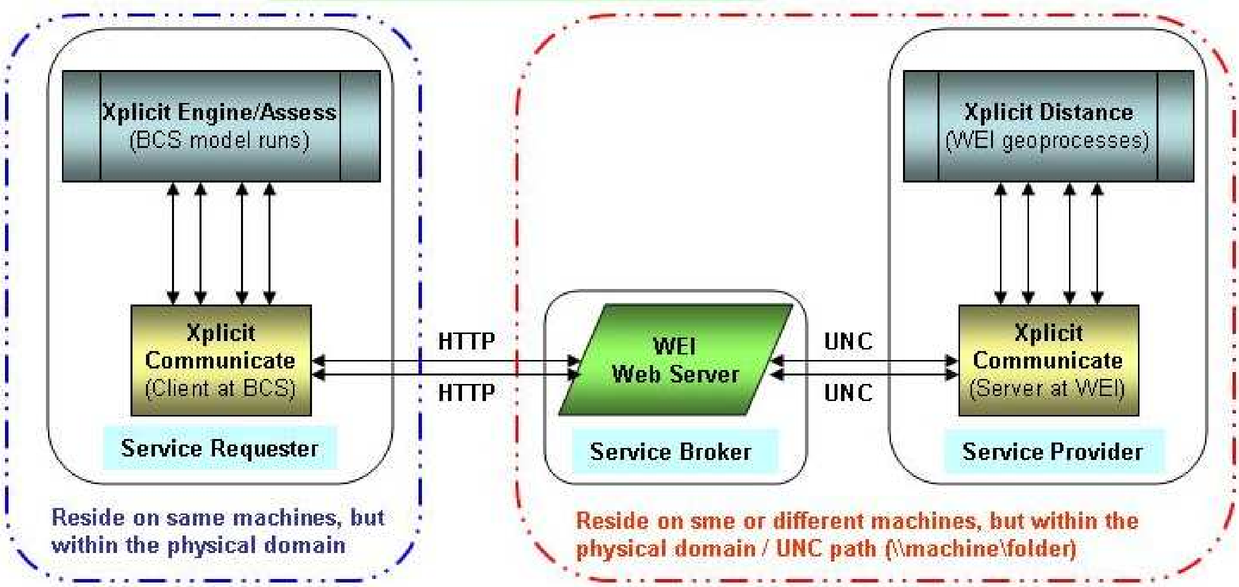


Figure 38: Web-service system architecture (*XCommunicate*) (in cooperation with R Vamshi (WEI), pers. comm.; WEI = Waterborne-Environmental Inc.).

5.3.5.7 Ecological Models

For the majority of species, regulatory protection goals require risk characterisation for the biological entities (meta-) population or community (Section 4.3), whereas ecotoxicological effect testing is basically done at individual level. A range of mathematical model approaches, referred to as 'ecological models' (or mechanistic effect models), exist which can support bridging that gap (*e.g.*, Pastorok *et al.* 2002, Suter 2007).

A prominent ecological model family are *Individual-Based-Models* (IBMs, or *Agent-Based-Models*, ABMs, (terms are used synonymously), Grimm & Railsback 2005, 2011). In an IBM, the system's individual entities and their behaviours are represented (*e.g.*, individuals of a population). "*Instead of describing a system only with variables representing the state of the whole system, we model its individual agents. ABMs are thus models where individuals or agents are described as unique and autonomous entities that usually interact with each other and their environment locally. Agents may be organisms, humans, businesses, institutions, and any other entity that pursues a certain goal. Being unique implies that agents usually are different from each other in such characteristics as size, location, resource reserves, and history. Interacting locally means that agents usually do not interact with all other agents but only with their neighbors—in geographic space or in some other kind of "space" such as a network. Being autonomous implies that agents act independently of each other and pursue their own objectives. … Hence, with ABMs we can study questions of how a system's behavior arises from,* *and is linked to, the characteristics and behaviours of its individual components.*" (Grimm & Railsback 2011).

In regulatory RA of PPPs, ecological models have been introduced at almost all biological organisation levels (*e.g.*, Toxicokinetic-Toxicodynamic Modelling (Ashauer 2012), ELINK (Brock *et al.* 2009), Pastorok *et al.* 2002, Suter 2007). The role of ecological models in ecological RA of PPPs with respect to Ecosystem Service is discussed by Galic *et al.* (2011). As of this writing, joint initiatives of research, authorities and industry are ongoing, aiming at guidance on the use of ecological models in regulatory RA and RM (*e.g.*, SETAC Europe Advisory Group on Mechanistic Effects Models for Risk Assessment (SETAC 2013), CREAM Marie Curie Initial Training Network ("Mechanistic Effect Models for Ecological Risk Assessment of Chemicals" (CREAM 2013), ModeLink (SETAC Europe Technical Workshop, October 2012, April 2013)).

The *Xplicit-Framework* is designed to (Section 5.3.4) operate with ecological models as *Associated-Models* (Section 5.3.4.10). As farmer behaviour, exposure and eFate of substances can largely be regarded as independent from species presence and their substance intake, a feedback loop of the outcome of an ecological model into these models between time-steps is not necessary. Thus, the ecological models can operate subsequent to eFate calculation. However, the framework allows also to take time-step dependencies into account (*e.g.*, for Non-Target-Terrestrial Plants, local plant mortality can increase subsequent spray-drift exposure of neighbouring plants).

In an example study (Section 6.4) the ecological model 'MASTEP' for *Asellus aquaticus* is linked to Xplicit. MASTEP is an IBM which operates spatiotemporally explicit, hence, expects spatiotemporally explicit PECsw (van den Brink *et al.* 2007, Galic 2012). In the *Xplicit-Aquatic-Model*, biological *Receptors* represent the biological entity and assessment attribute (Section 5.3.4.9) which are linked to abiotic *Receptors* representing water body segments. The biological *Receptors* hold the output of MASTEP (*e.g.*, abundance of *Asellus aquaticus*).

5.3.5.8 Outlook

The *Xplicit-Framework*, together with the *Associated-Models* introduced above, allow to address a range of current RA and RM problems (example studies, Section 6). However, as discussed in Part 1 (Section 4), in the context of forthcoming protection goals and RM problems, a range of challenging problems are ahead. Xplicit is designed to be adaptable to support the risk characterisation of such problems, *e.g.*, by developing and/or implementing the necessary *Associated-Models*. As of this writing, the following developments or adaptations of models to operate with the *Xplicit-Framework* are ongoing:

- Refined aquatic *Receptor* model: Water and sediment phase, and using a hydrological model which is based on water body network topology (with refined eFate processes).
- Exposure model: Mechanistic run-off filter modelling using the VFSMOD model (B Röpke pers. comm., IFAS 2012).
- Exposure model: Mechanistic spray-drift modelling using the model developed by Miller & Hadfield (1989). This model is capable to estimate spray-drift in dependence of weather conditions (*e.g.*, wind direction, wind speed, temperature, relative humidity) and agricultural conditions (*e.g.*, nozzle type, pressure, tractor speed).

- Exposure model: Empirical dust-drift model to estimate exposure of bee forage plants occurring in the vicinity of fields, due to deposition of active substance-containing dust from abrasion of (insecticidal) treated seeds.
- Effect model: A community model for Non-Target-Terrestrial Plants (NTTPs) to be linked to biotic NTTP-*Receptors*, in order to assess potential effects of herbicidal spray-drift depositions at Assessment Endpoints of the biological entity 'community' (May *et al.* 2009, Prof. F Jeltsch, University Potsdam, pers. comm., 2012).
- Effect model: Linking a terrestric-version of the MASTEP (meta-) population model approach for Non-Target-Arthropods to biotic *Receptors* in order to represent population-level Assessment Endpoints (*e.g.*, abundance, recovery) (Thorbeck P, Baveko H, presentation at SETAC Europe 2011, ModeLink Workshop, pers. comm.).

5.4 Ready-to-Use Models – 'Xplicit-Models and Scenarios'

Xplicit-Models are ready-to-use models for landscape-scale ecological risk characterisation. The user only has to parameterise a predefined configuration which can be done by using a common text editor or via web-browser in a web-server environment (Section 5.3.3.1, Figure 13, Section 5.3.4.2, Figure 18, Figure 19). *Xplicit-Models* are derived from the *Xplicit-Framework* by associating (external-) models and a configuration, which can technically require to write an adaptor (Section 5.3.4.10, using the Microsoft .NET Framework and *e.g.,* C#) and XML. Thus, an *Xplicit-Model* can be regarded as an 'implementation' or 'customisation' of the *Xplicit-Framework*.

An *Xplicit-Model* together with a specific parameterisation and specific data is called an *Xplicit-Model Scenario* (Figure 39). An *Xplicit-Model Scenario* intends to address a properly defined problem formulation. Example *Xplicit-Model Scenarios* are introduced in the case studies in Part 3 (Section 6).

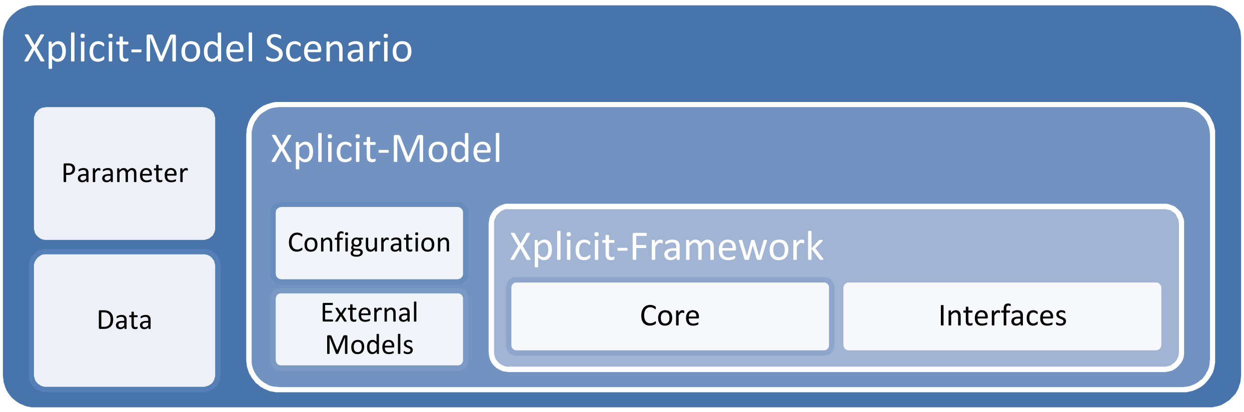


Figure 39: Schematic relationship between the *Xplicit-Framework*, an *Xplicit-Model* and an *Xplicit-Model Scenario*.

5.4.1 Simulation Process

In Part 1 (Section 4) landscape-scale approaches were discussed in the context of regulatory ecological RA and RM of PPPs. Results were transferred into the *Xplicit-Framework* development in Part 2 (Section 5). The purpose of an *Xplicit-Model* and *-Scenario* is typically given by a RA or RM problem, hence, by risk characterisation that matches protection goals. A typical Xplicit simulation process is illustrated in Figure 40 and is briefly discussed below (see also case studies in Part 3, Section 6).

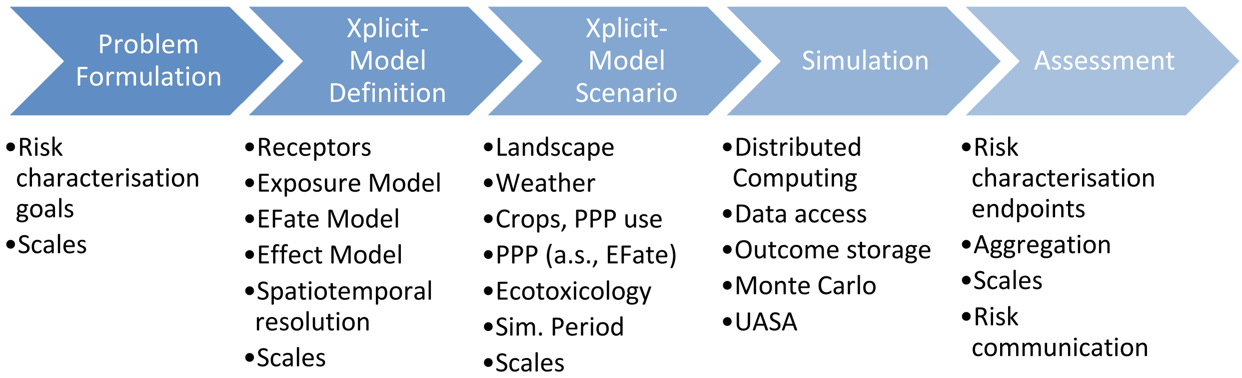


Figure 40: Main Xplicit simulation processing steps ('Sim.Period' = simulation period).

i. Problem formulation: A clear concept of the underlying questions or hypotheses to be addressed is needed. In regulatory RA of PPPs, questions can arise from lower-tier RA levels. Thus, the intended risk characterisation is related to regulatory protection goals (Section 4.3).

ii. *Xplicit-Model* definition: The structure of an *Xplicit-Model* is defined by its purpose, hence, by the RA problem formulation (and practical considerations) and consists of the *Xplicit-Framework*, *Receptors*, *Associated-Models* (Section 5.3.5) and their configuration (*e.g.,* considering scale dependencies using spatiotemporal signatures of PDFs).

iii. *Xplicit-Model Scenario* definition: Having defined an *Xplicit-Model* as an abstraction of the real-world system, building a scenario is necessary to address the problem formulation. In a landscape-scale assessment this is done in terms of defining, *e.g.,* the study region, its entities and discretisation, Assessment Endpoints, PPP use, eFate description, and further parameterisation. Again, scale dependencies are taken into account by defining spatiotemporal scales at which variability occurs. The scenario definition can make use of uncertainty assessment (UASA, Section 5.3.4.13).

iv. Simulation: The distributed computing environment (Section 5.3.4.14) is initialised. An *Xplicit-Management* (*XM*) instance in combination with the XML configuration and parameterisation file (*e.g.,* via web-browser) is started. *XM* prepares *Tasks* for *Xplicit-Processors* (*XPs*) and administers the simulations. A typical time-step calculation cycle is shown in Figure 41. In each time-step (*e.g.,* day or hour), *Associated-Models* are requested to do their calculations (*e.g.,* Section 5.3.3.3, Figure 17). Technically, resulting exposure ($PEC_{(r,t,a.s.)}$) and effect (*e.g.,* $Effect_{(r,t,a.s.)}$) matrices for each *Receptor* and a.s. are extended by a column in each time-step (illustrated in Appendix 11.4, Figure A 22). The resulting matrices represent a possible 'full picture' of exposure ($PEC_{(r,t,a.s.)}$) and effects (*e.g.,* $Effect_{(r,t,a.s.)}$) for each Monte Carlo, hence, build the basis of a possible statistically independent case for risk characterisation. Monte Carlo runs can be nested into an Uncertainty-Analysis/Sensitivity-Analysis (UASA, Section 5.3.4.13).

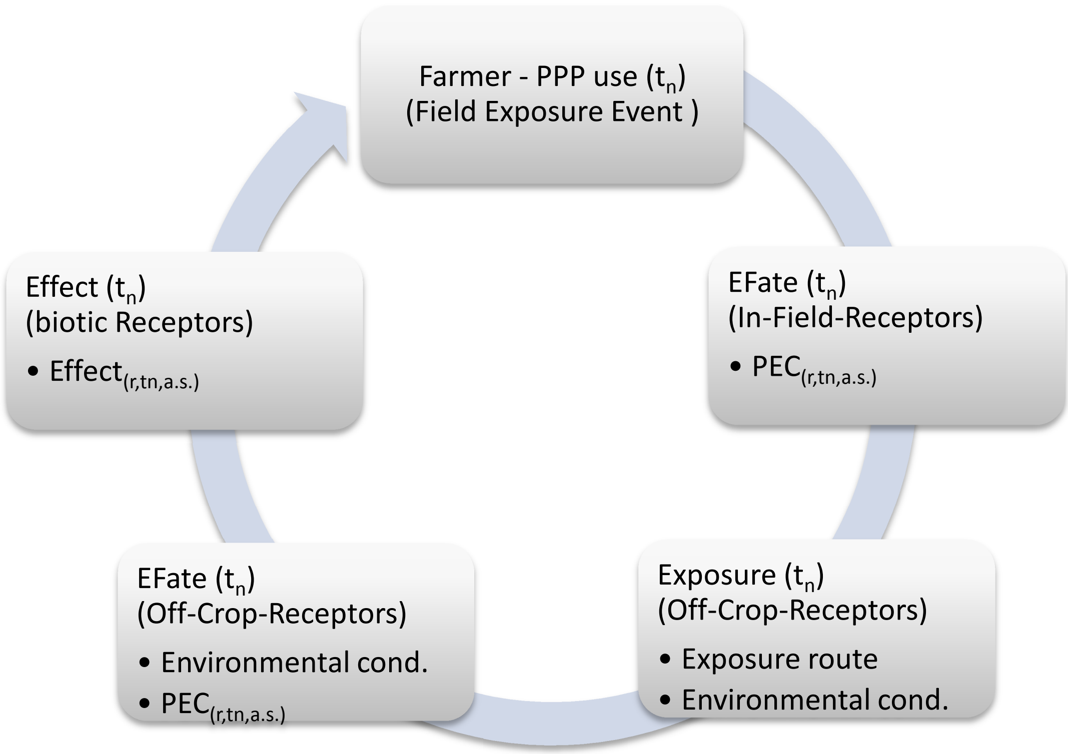


Figure 41: Schematic time-step processes. The field is the target unit of a PPP application event, hence, its (abiotic) *In-Field-Receptors* are initially exposed. *In-Field-Receptors* build the source of exposure modelling of *Off-Crop-Receptors*, which depends on actual environmental conditions ('cond.', *e.g.,* wind, rainfall). Exposure amounts reaching *Off-Crop-Receptors* (their compartments) are subject to eFate calculations (for which t_n and t_{n+1} calculations can be distinguished in case relevant to effect calculations). Biotic *Receptors* represent Assessment Endpoints (Section 5.3.4.9). PECs of *Off-Crop-Receptors* compartments are taken as input for corresponding effect models. In time-steps without PPP application events, only eFate and effect are calculated.

v. Assessment: Risk characterisation takes different risk dimensions into account, based on the 'full picture' data on exposure ($PEC_{(r,t,a.s.)}$) and effects (*e.g.,* $Effect_{(r,t,a.s.)}$), for each Monte Carlo run. Analysis can target at, *e.g.,* percentiles of PECs and effects of *Receptors* at different scales (*e.g.,* receptor-, habitat-, regional-scale) and their expectancy values, probability of exceedance of a given threshold value at different scales (*e.g.,* P(90th percentile PECsw > trigger)), fractions of habitat of a given condition (*e.g.,* fraction of Non-Target-Arthropod habitat of TER < 5), recolonisation potential (Section 6.1), or time-to-recovery (Section 6.4). Example analysis is presented with the case studies in Part 3 (Section 6). Spatiotemporally explicit results can be verified against straightforward spatial analysis (GIS) for risk potential. Results can be aggregated at different levels for adequate risk communication using visualisation methods (*e.g.,* web-mapping, dynamic time series, etc.).

The number of Monte Carlo runs necessary to produce a sufficiently accurate outcome (low confidence bounds) should be subject to investigation and will depend on the endpoint and its scale (*e.g.*, PECsw variability of a local water body segment will be much higher than a 90th percentile PECsw of all water body segments at landscape-scale).

5.4.2 Platforms

Xplicit-Models can be generally processed at any operating system running the Microsoft .NET Framework (Microsoft 2012b, version 4.0 or higher). This includes, *e.g.,* local Personal Computers, servers residing in a network, or the Microsoft Azure Cloud Computing platform (Microsoft 2013). These platforms were used in the example studies presented in Part 3 (Section 6). Data can be provided by a database, using files or web-services (Section 5.3.4.15).

5.4.3 *Xplicit-Model* Verification and Validation

5.4.3.1 *Xplicit-Model* Verification

As discussed in Section 5.2.8, model verification does not refer to the usefulness of the model with respect to address problem formulations in risk characterisation, but tests the system against the full range of functional and non-functional requirements (Section 5.2.3, 5.3.2) including technical aspects.

Xplicit-Model verification was partly covered by Unit-Tests (Section 5.2.8) done in the course of the *Xplicit-Framework* development (Section 5.3), yet, was explicitly done for the *Xplicit-Models* used in the case studies shown in Part 3 (Section 6). System-Tests ('Black-Box-Tests', Section 5.2.8) were conducted manually with a range of parameterisations and data. Besides key functionality (*e.g.*, initialisation, Monte Carlo, distributed computing, data input/output, scale-dependent PDF sampling, co-operation with *Associated-Models*, etc.) and quality attributes (*e.g.*, resources, runtime, scalability), major elements of the *Xplicit-Model* verification was the evaluation of its outcome with respect to correctness of calculations (*e.g.*, PEC, effects). At first glance it may appear that checking 10^n values produced by a probabilistic model, based on large datasets, is hardly ever possible. However, in landscape-scale approaches outcome is related to spatial units, hence, can be mapped. Mapping of, *e.g.*, PEC(r) or Effect(r), overlain by additional spatial data, if supportive, provides an immediate visual impression of plausibility of values. Likewise, maps for time series can be generated and inspected in their dynamic behaviour, when run as movies. This 'visual debugging' is a major tool for verification of quantitative outcome. Visual pattern can also provide an impression on how the model has employed variability at different scales. From the mapped outcome, samples can be drawn (randomly or subjectively) and can be re-calculated manually by using the input data and model approaches. For example, for spray-drift entries into water bodies, initial PECsw and resulting effects can be checked using spread-sheet calculations.

Ultimately, Unit- and System-Tests ('Black-Box-Tests', Section 5.2.8), including 'visual debugging' of model outcome, can allow the statement that an *Xplicit-Model* has been verified against exactly this test environment. Model verification comes therefore with a statistical certainty, which is expected to increase with model use in further risk characterisations.

5.4.3.2 *Xplicit-Model Validation*

Model validation is generally regarded as a quality attribute for the use of a model in regulatory decision-making; however, 'model validation' is a term that requires clarification.

Xplicit-Model validation is related to *Xplicit-Model-Scenarios* (above) which build the basis to address a RA problem formulation. The straightforward question of whether the model correctly represents (or reproduces) the behaviours of the modelled real world system can hardly be answered, as the model is a (drastic) simplification of the real-world system, and as present (or past) experience and data are part of the model scenario assumptions (*e.g.*, environmental and agricultural conditions). Variability and uncertainty of the latter led to the use of probabilistic methods causing outcome comparison to real-world conditions to require considerable spatiotemporal sampling density in practice (*e.g.*, the EUPRA workshop recognised that comprehensive validation is probably unachievable, Hart 2001). For example, assessing an *Xplicit-Model* for aquatic exposure (*e.g.*, Section 6.3 and 6.4) against empirical monitoring data, with reasonable statistical significance, would require correspondingly intense spatiotemporally sampling. Methods of pattern comparison between predictions and observations in space and time can provide more relevant statements on model validation than individual point comparisons (Grimm & Railsback 2011). In this context, pattern can be regarded a higher-scale comparison level than the individual point level. With increasing predictive power of landscape-scale risk characterisation, the question of validation gradually moves towards the question of whether the model reproduces real-world system behaviour.

Therefore, the question of validation needs to be specified in context of the model purpose, and its ultimate goal is more to assess the model (scenario) usefulness in addressing the problem formulation. Thus, model validation is regarded in the spirit of the well-known statement of George Box, "*Essentially, all models are wrong but some are useful*" (Box 1979).

A useful model can be regarded to support decision-making in a Bayesian view (Section 4.3.1.1), *i.e.*, as a contribution to improve the overall knowledge upon which risk characterisation and decision-making are based. In this view, the model does not make the decision in a sense that its outcome inevitably causes a certain decision, it rather supports the decision-making. For example, in RM question of where to invest windbreaks as a shelter of water bodies against spray-drift, an *Xplicit-Model* can be a useful model to characterise risk of WB segments and water bodies (*e.g.*, case studies Section 6.3 and 6.4). In the ultimate RM decision, the outcome of the model might be directly implemented, yet, can be used as a contributor in addition to further knowledge sources and expert judgement. Therefore, for purposes of risk characterisation in regulatory context of PPPs as discussed in Part 1 (Section 4), model validation can be interpreted as to whether the model (scenario) "*makes a reliable and* *quantifiable contribution to reduce the overall uncertainty in ecological risk characterisation and decision-making*".

Particular difficulties for model validation in regulatory RA context arise from the fact that in the tiered risk characterisation approach (Section 4.3.2) the model scenario is basically defined to be conservative, hence, its predictions can hardly be validated against empirical observations (except those having a correspondingly large dataset). For example, spray-drift deposition was intentionally measured at conservative wind conditions with respect to Good Agricultural Practice and without spray-drift filtering elements (Rautmann *et al.* 2001), hence, the purpose of these data as a conservative basis has to be taken into account in validation of a spray-drift variability model derived from these data (*e.g.,* Schad & Gao, Section 5.3.5.4, Golla *et al.* 2011). In context of SPGs (Section 4.3.2), reference scenarios are to be developed for the purpose of more realistic, yet, still protective risk characterisation. This will define also the context for validation of a model operating at this RA tier.

The Bayesian view of the role of a model in regulatory decision (above) points out, that introducing a model into the knowledge building process indicates that models were already there, yet, in terms of less explicit and quantitative mind models or expert judgement. The usefulness of the model has to be judged on the purpose to get a more solid knowledge base than without the model.

On this background, validation could include different steps, *e.g.,*

- model verification (above),
- scientific review of model concepts and approaches (*e.g.,* 'process validation') with particular review of *Associated-Models* (*e.g.,* exposure, eFate),
- scientific review of scenario assumptions, including data validation (*e.g.,* geodata 'ground truthing') or the eFate behaviour of active substances,
- scientific review of model reliability ('behaviour') regarding propagation of variability and uncertainty to model outcome in the context of risk characterisation problem formulation ("*how does the model relate to expert knowledge?*"), including a Sensitivity Analysis, SA),
- if possible, definition of test-scenarios for validation (*e.g.*, compare to FOCUS 2001).

The model and its scenario would then be considered as being validated against these test criteria.

5.4.3.3 Sensitivity Analysis

The robustness of the results of an *Xplicit-Model* can be assessed in a *Sensitivity Analysis*. A *Sensitivity Analysis* appoints uncertainty in the model output to sources of uncertainty inputs, thus intends to understand relationships between model input parameters and its output (*e.g.*, Saltelli *et al.* 2000). *Sensitivity Analysis* is closely related to *Uncertainty Analysis* (*Uncertainty-Analysis/Sensitivity-Analysis*, UASA). A 2nd-order Monte Carlo approach has been implemented to conduct UASA (Section 5.3.4.12).

Sensitive model input parameters (and data) should be subject to particular attention in the model verification and validation process (*e.g.,* identifying necessity for further research). In contrast, less sensitive parameters could be removed from the model processes.

The results of a model *Sensitivity Analysis* can play an important role in model communication, hence, in respect of perception and credibility of a model in a regulatory context. *Sensitivity Analysis* should be part of the procedure for establishing *Xplicit-Models* in regulatory RA and RM.

5.4.3.4 Review

The development of the *Xplicit-Framework* and the use of *Xplicit-Models* in risk characterisation problems (Section 6) was accompanied by an exchange process which covered different aspects and included experts from different institutions (*e.g.,* internal Bayer CropScience modeller and risk assessors, Institute of Environmental Science at University Koblenz-Landau, Ghent University (Dept. of Mathematical Modelling, Statistics and Bioinformatics), authorities (*e.g.*, German Federal Environment Agency (UBA), UK Chemicals Regulation Directorate (CRD)), and the scientific community (Schad & Schulz 2011, presentations at different occasions *e.g.*, at SETAC Europe, Schad 2009, Schad *et al.* 2011).

The review process aimed at critical discussion of the Xplicit concepts and approach, the model requirements definition and their fulfilment, its use in specific RA problems and potential needs for future development.

In summary, as of this writing, the review process has resulted in a general agreement on the identification of the necessity for such a landscape-scale explicit and probabilistic approach. Also, the basic objectives, concepts and model approach of Xplicit were basically agreed. Xplicit was regarded a valuable approach to improve realism in RA and RM questions. Regarding the use in regulatory RA and RM, a need for guidance and harmonisation of landscape-scale approaches was identified, as well as for the development of standard scenarios for ecological RA. In particular, the definition of detailed criteria on risk acceptability in different risk dimensions was identified as necessary (development of SPGs, Section 4.3.2), with some emphasis on further influences to populations (stressors) occurring at landscape-scale (Section 4.4.2). Moreover, detailed risk characterisation will require to improve risk communication tools and skills, as well as harmonisation (Section 4.3.1). Results of the review have been considered in the development process and were considered in the outlook (Section 5.5).

5.4.3.5 Failure Modes and Effects Analysis

In regulatory RA of PPPs, false model predictions could have significant adverse effects on decision-making regarding RM. Ecological risk could be overestimated ('false positive') with the consequence of ineffective RM and unnecessary cost, or worse, could be underestimated ('false negative') with the consequence of unacceptable real-world ecological effects. Besides such far-reaching impacts in model use, software errors, ranging from conceptual to coding errors, can lead to significant cost.

Failure Modes and Effects Analysis (FMEA) is a general failure analysis method to identify system failure modes and to assess their possible impacts (and their likelihood to occur) (wikipedia.org, Behrmann 2012). Failure modes early identified in the system development process are generally considered to lead to lower cost than such identified at late stages or even in operation.

In the development process of the *Xplicit-Framework* and with respect to *Xplicit-Models* and their use in regulatory risk characterisation, basic principles of FMEA were considered (Section 5.2.2) in order to establish a permanent awareness on possible errors and their consequences. This awareness contributed to, *e.g.*,

- concepts to manage complexity, *e.g.*, Modularity, service-orientation (Section 5.3.2, 0 and 5.3.4);
- implementation using Object-Oriented-Programming;
- model verification (*e.g.,* Unit-Tests, System-Test, Section 5.4.3.1);
- *Xplicit-Model* use:
    - Experienced users: an *Xplicit-Model* is used by experienced (trained) modellers.
    - Study directors have the full responsibility in their domain, which requires a good understanding of the tools used and how they are used (*e.g.*, input (geo)data quality check, process log-files, evaluation (*e.g.*, visualisation, check against straightforward spatial analysis using standard GIS), reporting) - "*each model runs with senseless input, especially scientific ones*" (anonymous).
    - Integrative use in risk characterisation: *Xplicit-Model* outcome is part of a tiered risk characterisation scheme with a range of data available to the risk assessor.
    - RA which uses *Xplicit-Model* outcome is done by experienced risk assessors who are able to assess the reasonability of a risk characterisation.

5.5 Outlook

Xplicit-Model-Scenarios represent the ultimate product of the Xplicit development, which is applicable to RA problems. Improving the direct applicability of *Xplicit-Models* and *Xplicit-Model-Scenarios* is a key objective of ongoing developments. Ultimately, the user should be enabled to conduct *Xplicit-Models* via web-browser, without the need for software installation or (geo)data acquisition. This process will be accompanied by *Xplicit-Model Sensitivity Analysis* to which technical prerequisites have been established.

Associated-Models and *–Services* represent the processes and data of *Xplicit-Model-Scenarios*. Improving the predictive power requires to introduce further processes and data into *Associated-Models*. This is envisaged for risk characterisation of aquatic organisms by introducing hydrological and more detailed eFate models, ecological models (*e.g.*, MASTEP, Section 5.3.5.7), as well as more detailed exposure models for run-off (*e.g.*, FOCUS 2001, VFSMOD, B Röpke pers. comm., IFAS 2012). The current *Landscape-Metric* service (Section 5.3.5.2) can be improved by further automation in order to establish an *ad hoc* service endpoint. Geoprocessing services for assessing the outcome of Xplicit simulations can further improve risk characterisation and risk communication (*e.g.*, by visualisation). *Associated-Models* depend on empirical evidence (*e.g.*, spray-drift deposition, Section 5.3.5.4). Feedback from landscape-scale (Xplicit) modelling, especially with respect to scale-dependencies of processes, into data generation efforts is regarded important to improve the underlying databases and corresponding models.

An important insight resulting from the evaluation process of landscape-scale modelling in risk characterisation (Section 4.5) was to separate disciplines and not to establish a silo-like complex model. The *Xplicit-Framework* modules are a step in this direction. The vision behind this development is that basically any entity that provides a (key) service to a landscape-scale risk characterisation can be represented by a service endpoint with clear specifications, and hence, can reside anywhere in a network, employed by a central model unit. A layered system could be established comparable with such of a network communication system (Open Systems Interconnection (OSI), Wikipedia.org). Having clear contracts agreed ('Service-Level-Agreement'), the actual risk characterisation modeller or risk assessor does not need to practically deal with, *e.g.*, geodata, hydrological modelling or representation of species in an ecological model.

Xplicit-Models and *–Scenarios* can make valuable contribution at different levels of regulatory risk characterisation of PPPs: (i) Xplicit can support scenario development for different RA tiers by quantifying protection levels, (ii) *Xplicit-Models-Scenarios* can be employed at future standard tier RA levels (*e.g.*, 'reference scenario', EFSA 2010a), and (iii) as higher-tier approaches (Part 3, Section 6). Employed as a higher-tier approach, Xplicit indicates the necessity and fields for harmonisation, whereas at lower-tier *Xplicit-Models-Scenarios* can make significant contribution to harmonisation.

6 Part 3: Xplicit in Risk Characterisation Studies

This section presents case studies from different fields of ecological RA and RM for Non-Target-Organisms in regulatory context of PPPs. Case studies provide a good means to verify the Xplicit concepts and approach from an applied viewpoint, to show its potential and to identify areas for improvement. Beyond this, the presented problem formulations, results and conclusions provide first examples of refined risk characterisation. Some studies were conducted for Bayer CropScience PPPs. Thus, data related to business confidentiality have been anonymized which does not limit their use herein. The case studies do not claim to represent final conclusions on regulatory RA or RM measures. Each case study starts with a summary on the lessons learned with respect to the goals of this thesis.

In Figure 42, the Xplicit application scope is summarised as it has been explored so far. The generic design allows to apply the Xplicit concepts and approach to a range of risk characterisations of comparable structure and thus, to a range of RA and RM problems.

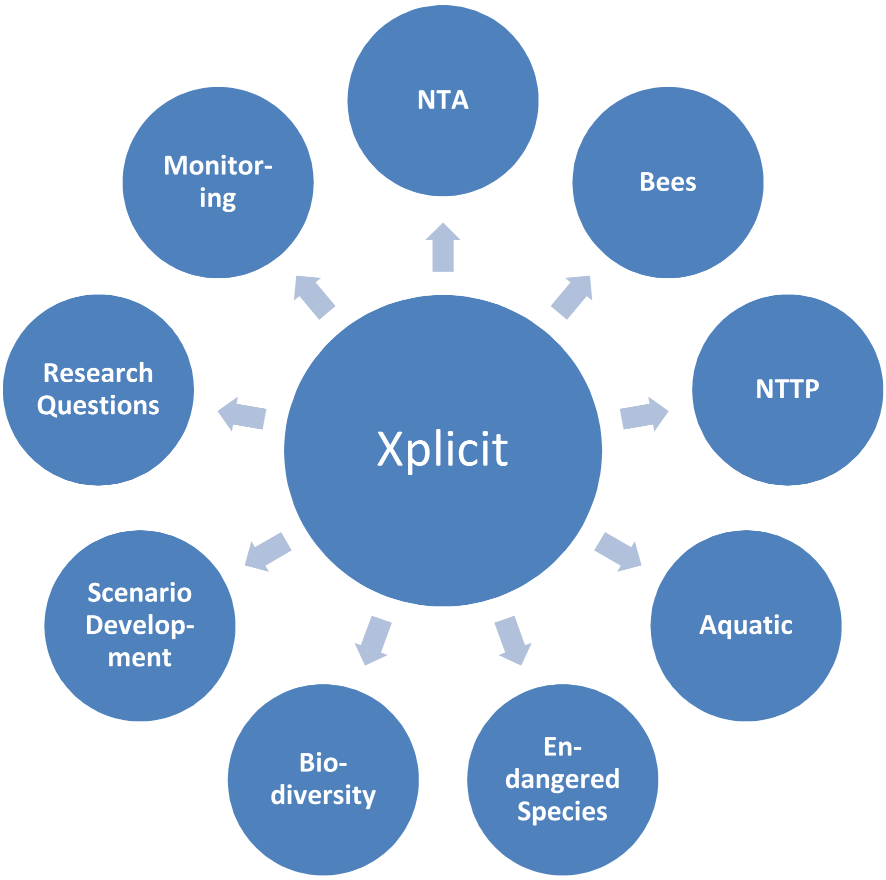


Figure 42: Xplicit application scope.

6.1 Risk Characterisation for Non-Target-Arthropods

A landscape-scale risk characterisation for Non-Target-Arthropods (NTA) due to spray-drift entries was conducted for hops and apple cultivations in Germany using the Xplicit approach. The study was among the first studies conducted using Xplicit and carries major aspects of landscape-scale risk characterisation, *e.g.*, stepwise refinement, importance of scales, scenario development (Section 4.4 and 4.5). Therefore, its presentation herein is extended and differs from other case studies.

The following sections provide the lessons learned with respect to the objectives of this thesis, as well as a concise presentation of the study objectives, methods, results and conclusions.

6.1.1 Lessons Learned

- The Xplicit approach allows to quantify spatiotemporal extent of exposure and effects at ecologically relevant scales, and thus, to set the definitions of the Tier-1 scenario in context to real-world conditions. This provides a new basis for RA and RM. Results can provide a basis for generic RM (*e.g.*, landscape management).
- The Xplicit approach allows to improve understanding of risk of Non-Target-Organisms by step-wise incorporating more risk driving factors and real-world context: In the case study, more realism was introduced by using real-world geodata on habitats and fields and by calculating exposure based on their spatial relation. The effect characterisation was kept at a simple Tier-1 TER level approach. The next step is proposed to consider mechanistic population modelling (Section 5.3.5.7) to transfer individual-level effects to population level.
- The study emphasises the importance of scale in risk characterisation. The topic of scale affects all aspects from the representation and processing of variability (and uncertainty), up to the evaluation of outcome and the communication of risk. Scales in the study range from local habitat segments, over individual habitats to cultivation regions and the country scale.
- Scale-dependent uncertainty propagation: Preliminary results suggest that variability (uncertainty) can be partly 'assimilated' in systems of hierarchical scales. Having defined the RA and RM decision scales (*e.g.*, regional scale), local parameter uncertainty can be 'trapped' in the scale it occurs, hence, is only partly propagated to ecologically relevant scale(s). Thorough research on these preliminary findings is proposed.
- The study provides an example on how representative scenarios (study regions) for refined risk characterisation can be derived by using metrics that quantify landscape composition and structure, and on how regional-scale results can be set in context to the country-scale (definition of Reference Scenarios, SPGs, EFSA 2010a). The stepwise introduction of ecological context was exemplarily shown in the assessment of recolonisation distances (*Aut-/SynContext*, Section 4.2).
- Xplicit has shown its applicability in refined ecological risk characterisation, to provide a quantitative basis for RA and RM. This comprises the implementation of an *Xplicit-NTA-*

Model, preparation of geodata as a *Landscape-Metric* service, processing simulations (*Xplicit-Engine*) and evaluation and reporting of outcome (*Xplicit-Assess*).

- Calculation of recolonisation distances demonstrated the value of modularisation and service orientation by employing a remote spatial processing service in the evaluation of Xplicit simulation outcome. This way, the Xplicit *Component Xplicit-Assess*, can modularise its different assessment aspects.
- Xplicit can run at the Microsoft Azure cloud computing platform. Parts of the Xplicit simulations were conducted at Azure (*Xplicit-Processors*, Section 5.3.4.3, with data at SQL-Azure, Microsoft 2013, Community Technology Preview (CTP), 2009, 2010, Dariusz Parys (Microsoft), Karin Sondermann (Microsoft), pers. comm.). This processing option underlines the scalability of the Xplicit modelling framework.

6.1.2 Extended Abstract

A landscape-scale risk characterisation study for Non-Target-Arthropods (NTA) due to spray-drift entries of a PPP ('PPP-1') into their terrestrial habitats was conducted for hops and apple cultivations in Germany. The assessment was based on a refined characterisation of the co-occurrence of hops and apple cultivations with NTA habitats ('off-crop') using geodata combined with a spatiotemporally explicit exposure modelling approach (Xplicit).

The standard Tier-1 RA indicated a concern for NTAs in the off-crop area and the need for a refined RA (Toxicity Exposure Ratio, TER < 5, the required trigger). The Tier-1 scenario for spray-drift assumes direct crop-habitat adjacency, unprotected downwind location of habitat, 90th percentile spray-drift deposition without consideration of the recovery potential. However, actual adjacency of cultivations and off-crop play a decisive role for spray-drift exposure. An off-crop area which is not in direct vicinity of a treated field is exposed less than an off-crop area which borders on a field. Size and connectivity of off-crop patches allow for recolonisation of potentially affected locations. Whilst the Tier-1 exposure scenario is protective, an exposure assessment which is based on realistic land use and land cover configuration is valuable to quantify potential risk more realistically.

Potential exposure of NTAs resulting from spray-drift for the use of PPP-1 in hops and apple cultivations in Germany was analysed with respect to the spatial composition of intensive crop cultivation regions. These regions had been chosen conservatively according to analysis of cropping data and the occurrence with off-crop. Geodatabases with a high spatial resolution were developed that contain a detailed characterisation of the local environmental conditions in the off-crop surrounding of hops and apple cultivations. The development process was accompanied by a field observation.

The key component of the study was the refined risk characterisation for NTAs performed in regions of intensive co-occurrence of cultivations and off-crop ('Study Regions', 'SRs'). In a second part, results obtained for the SRs were set in context to the conditions in the entirety of cultivations in Germany ('context-setting'). Particular attention was paid to the characterisation of the spatial and temporal extent of off-crop areas of TER < 5 and their connectivity to areas of TER ≥ 5, as well as to the question to whether TER < 5 areas might show spatial aggregation.

The SRs were determined with the aim to identify regions of high co-occurrence of the target crop (hops or apple) cultivations and off-crop, hence, of high potential of off-crop to be exposed due to spray-drift from PPP application on target crop fields. To this end, a Germany-wide dataset was developed based on the ATKIS database. Off-crop was defined as land cover of particular importance for NTAs (*e.g.*, wood margins, groves, grasslands, riparian vegetation, etc.). Germany was divided into parcels of 2 x 2 km size. For each cell a co-occurrence index was calculated that combines the relative areas of target crop cultivations and off-crop (*CoOccInd*). *CoOccInd* is an indicator for the potential exposure of off-crop due to spray-drift from target crop cultivations: the higher *CoOccInd* the higher the potential spray-drift entries. SRs were determined to predominately contain grid cells from the upper ranks (>90th percentile *CoOccInd*) and coherent SRs were delineated.

The refined landscape-scale risk characterisation was done on the basis of two SRs for hops (Hallertau) and five SRs for apple cultivations (Lake Constance, Saxony). The crop-specific SRs in total provide a conservative representation of the potential of NTA habitats ('off-crop') to be affected from spray-drift entries for the use of PPP-1 in the target crop cultivations. In total, the SRs cover an area of >13,200 ha for hops and >27,600 ha for apple cultivations. Characterisation of the occurrence of cultivations and off-crop was done using high-resolution (hres) aerial imagery. The SRs for hops contain ≈3,200 ha of hops cultivations with ≈2,600 ha off-crop, those for apple contain ≈6,000 ha of apple cultivations with ≈6,600 ha off-crop. In order to assure a conservative assessment, refined risk characterisation for NTA was limited to an outer margin of off-crop habitats (*e.g.*, for wood, only the wood margin was assessed).

Compared to the standard Tier-1 EA scenario the following factors were refined: landscape structure; local crop – to – off-crop distance; variability of wind directions; variability of local spray-drift deposition.

For the RA, TER values were calculated based on expectancy values of 90th percentile PECs (<P90 PEC>) and the lowest ecotoxicological endpoint from the Tier-1 RA level (effects on reproduction). Since the endpoint was derived in a 2-dimensional test system a vegetation dilution factor of 5 (German regulations) has been considered. A TER ≥ 5 indicates that no unacceptable adverse effects on NTA species are to be expected. TER assessment was performed for each receptor at each time step in order to, *e.g.*, estimate probabilities of TER violation (TER < 5) or fraction of off-crop of TER violation. The number of Monte Carlo runs conducted depended on the stability of the key outcome. Dissipation of the active substance of PPP-1 was defined as DT50 = 4.5 days.

For the use of PPP-1 in hops, a single application was assessed. For the use in apple cultivations, a twofold application with a 14 days minimum spray interval was assessed. A 7 days application window was assumed for each individual application, *i.e.*, all fields in a SR were applied within 7 days. The use of 90% drift-reducing technology was assumed, without an in-crop buffer as additional mitigation measure.

The refined risk characterisation at regional-scale shows that limited fractions of NTA habitats are expected to indicate TER violation (TER < 5, '<f_offCrop>'): <f_offCrop> = 3.5% for hops, <f_offCrop> = 6.8% for apple cultivations. Considering the 90th percentile (P90) as a realistic worst-case exposure value, TERs >> 5 result for both uses (hops, apple) which shows that to a large extent NTA habitats are unlikely to receive spray-drift entries leading to unacceptable risk.

In order to further assess the spatial and temporal dimension of risk, so called recolonisation distances were calculated. This analysis provides information on 'how far a species might need to travel' to recolonise a habitat fraction that has received a TER < 5, and 'how long it takes' until such a habitat fraction can be recolonised (*i.e.*, has again a TER ≥ 5, due to dissipation of the a.s.). The results show, median recolonisation distances are 4.2 m (90th percentile (P90) recol.-dist. = 16.6 m) for hops, and 5.3 m for apple cultivations (P90 recol.-dist. = 21.2 m). The results (Section 6.1.5) allow for the following risk characterisation at landscape-scale:

i. NTA habitat fractions of TER < 5 are to a large extent well connected to habitat fractions of TER ≥ 5, which indicates a generally high recolonisation potential between potentially effected habitat fractions and refuges.

ii. Recolonisation can mostly occur from within the same NTA habitat patch that has partly received exposure leading to TER < 5, *i.e.,* refuges mostly exist in the same habitat.

iii. The findings in (i) and (ii) demonstrate that, spatial aggregation of risk is unlikely.

For the characterisation of the temporal dimension of risk, temporal recolonisation 'distances' (in [days]) were assessed: For both crops, the median temporal recolonisation distance are about 6-7 days (P90 temporal recol.-dist. = 12.5 days for hops and 15.2 days for apple cultivations). These results show that the violation of the TER = 5 threshold (referring to reproduction effects of the most sensitive species) are temporally limited to about 1-2 weeks after PPP-1 has been used in all hops/apple fields.

Among the off-crop types occurring in the cultivated landscape, wood margins, grassland (meadow, pasture), meadow orchards, groves, hedges and related types show highest levels of protection (numerically shown *e.g.*, in TER values >>5). For off-crop type 'herbaceous' the highest habitat fractions of TER < 5 were obtained. This is in agreement with intuitive expectation as the type herbaceous often occurs in direct vicinity of fields. For the risk characterisation of NTAs it has to be taken into account that herbaceous habitats account for about <10% of NTA habitats in total, and that 'herbaceous' is mostly represented by comparably small areas often occurring as strips between fields and roads, and so, are typically affected by various anthropogenic impact (*e.g.*, fertiliser, maintenance).

Aggregation was not only investigated at the scale of the individual NTA habitat but also at regional scale: Areas of TER < 5 occur in the vicinity of field boundaries, hence, can only occur according to the spatial distribution of local field-to-off-crop co-occurrence. As these co-occurrences are spatially distributed across the landscape, at regional scale, there is limited potential for aggregation.

The findings of the detailed landscape-scale risk characterisation obtained for the SRs were set in context to the country level by means of landscape metrics, well-established in landscape ecology (McGarigal & Marks 1995, McGarigal *et al.* 2002, Leitao *et al.* 2006). The results of the context-setting analysis consistently support the conservative character of the SRs, hence, emphasise the protective character of the study results and conclusions drawn for the SRs. It was shown for both crops that

i. for the majority of cultivations in Germany outside the SRs the potential of off-crop to receive significant spray-drift from the use of PPP-1 leading to TER < 5 is in the main lower than for the SRs,

ii. off-crop areas of TER < 5 occur distributed in the landscape and are mostly interspersed by or connected to off-crop of TER ≥ 5, hence, aggregation is unlikely to occur,

iii. due to the size and extent of off-crop patches and their connectivity, as well as the interspersion of areas of TER < 5 and TER ≥ 5, the potential for recolonisation is generally high.

The risk characterisation of NTAs can be significantly improved by assessing the exposure potential due to spray-drift at landscape-scale. The refined RA is mainly a result of the real-world spatial relationship between the target crop (hops or apple) cultivations and off-crop, the composition and configuration of land use/cover and the variability of local spray-drift depositions. Together, these 'landscape factors' can be regarded as representing naturally present mitigation. Refined exposure assessment was introduced into TER RA with an effect endpoint based on the reproduction assessment with the most sensitive species and taking a TER of 5 into account.

As the results show, under field conditions the spatial and temporal extent of TER violation (TER < 5) is clearly limited. Correspondingly, the occurrence of the conditions of the Tier-1 scenario of spray-drift exposure is limited. Beyond the refined exposure assessment, it was shown that NTA habitat areas of TER < 5 are generally well connected to areas of TER ≥ 5 which can be regarded as refuges for recolonisation. It was also demonstrated that these results were obtained for regions of intensive co-occurrence of cultivations and off-crop (SRs), and so, the results are considered protective for the country level.

6.1.3 Introduction & Objectives

In the regulatory context, RA of PPPs for Non-Target-Organisms generally follows a tiered approach. At lower tiers, worst-case conditions are assumed in the ecotoxicological effect and in the exposure assessment, whereas more realistic conditions of real-word exposure and *e.g.,* population recovery are taken into account in higher-tier assessments.

The standard Tier-1 RA for NTA for the use of PPP-1 in hops and apple cultivations in Germany indicated a concern for NTAs in the off-crop area (TER < 5, the regulatory required trigger) and the need for a refined RA.

A landscape-scale exposure assessment built the basis of the refinements, whereas the characterisation of effects to NTAs was kept at lower-tier conditions, and so, the refined exposure assessment was set in relation to a lower-tier effect assessment (TER approach with TER = 5 trigger). Landscape-scale exposure and RAs provide the opportunity to study the spatial and temporal extent of risk, and so, contribute to better assess the acceptability of potential effects in the context of regulatory protection goals.

Refined risk characterisation for NTAs should be performed in regions of intensive co-occurrence of cultivations and off-crop ('Study Regions', 'SRs'). Results obtained for the SRs were set in context to the conditions in the entirety of cultivations in Germany. Particular attention should be paid to the characterisation of the spatial and temporal extent of off-crop areas of TER < 5 and their connectivity areas of TER ≥ 5, as well as to the question as to whether TER < 5 areas might show spatial aggregation.

6.1.4 Data and Methods

An 'extended summary' on data and methods underlying the study is provided to present more detailed information which is not shown in the Extended Abstract above.

6.1.4.1 Characterisation of Crop – to – Off-crop Co-occurrence

Landscape-scale exposure and RA requires adequate characterisation of land use / cover (LULC). This was achieved in a two-step approach:

1. Preparation of German-wide LULC data in medium-resolution (mres, ATKIS); purpose:
    a. Identification of conservative SRs to be investigated in high-resolution (hres).
    b. Context-setting of landscape-scale RA results obtained for SRs.
2. Development of LULC geodata for SRs in hres as a basis for detailed landscape-scale RA using a spatiotemporally explicit model (Xplicit).

6.1.4.2 Topographic Data

The official topographical database from ATKIS (Authoritative Topographic-Cartographic Information System, BKG 2006) with a scale varying from 1:5,000 to 1:25,000 was used. This information enables for deriving a largely comprehensive dataset on land use/land cover.

Four off-crop classes which are present in apple and hops cultivation regions were differentiated: (i) *wood margin* (ecotone is considered because it differs from core wood with respect to diversity and abundance of species; conservative definition as wood patches cover large areas, significant exposure due to spray-drift will not occur in core wood and a dilution effect is prevented); (ii) *groves, bushes, hedges, shrubs* (tree rows, hedges or small clusters of trees and bushes were considered separately; linear geo-objects (e.g. hedges) were buffered to obtain their spatial extent); (iii) *meadow margin* (conservative, as limitation to a margin overrates risk); (iv) *vegetation around water bodies* (linear water bodies were buffered to obtain their spatial extent).

6.1.4.3 Site Selection

The objective of the site selection process was to identify both conservative and coherent SRs for detailed exposure and effect assessment from the perspective of the entirety of hops/apple cultivations in Germany. By using the co-occurrence index (Equation 10), SRs with a high co-occurrence of hops/apple cultivation and off-crop were identified. The index was calculated on the basis of the ATKIS dataset for 2x2 km grids, and is considered an adequate indicator for the potential exposure of off-crop due to spray-drift from hops/apple cultivations: the higher the *CoOccInd*, the higher is the potential of spray-drift entries (Figure 43):

Equation 10: $\boldsymbol{CoOccInd_i}$ =

$$(\Sigma_j \, area_{crop\_ij}) \cdot (\Sigma_k \, area_{offCrop\_ik}) \, / \, (max_{l=1 \ldots N}(\Sigma_j \, area_{crop\_lj}) \cdot max_{m=1 \ldots N}(\Sigma_j \, area_{offCrop\_mj}) \,)$$

with: *CoOccInd* = co-occurrence index (0,1); i,l,m = index of the 2x2 km grid cells; j,k = index of individual LULC polygons within a certain grid cell; N = total number of grid cells containing crop (specific number for hops and apple).

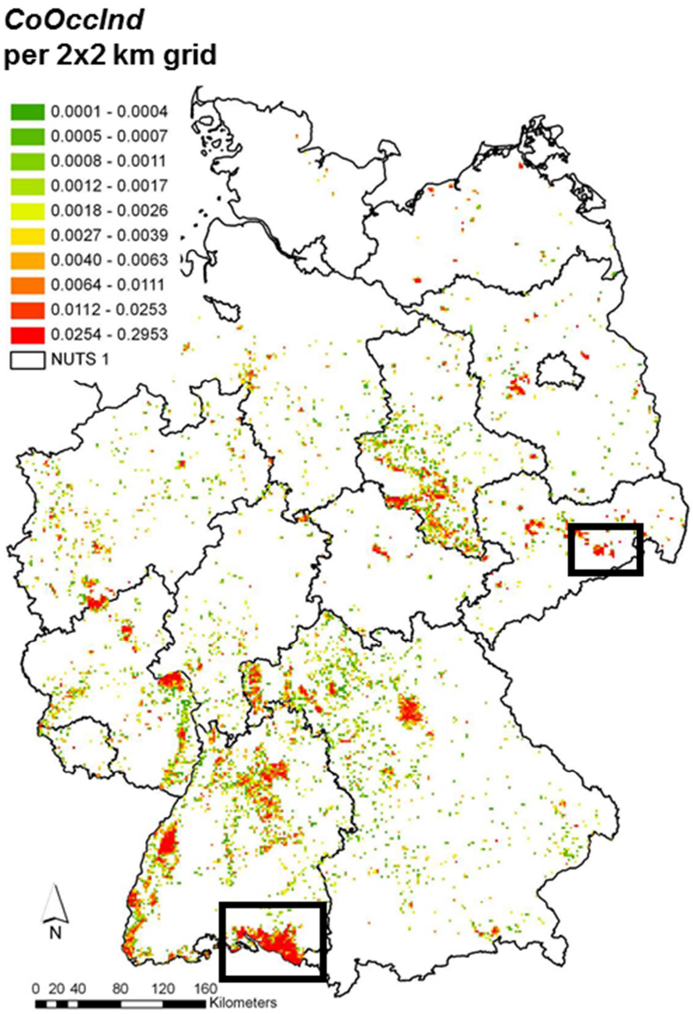


Figure 43: Co-occurrence index for apple, based on ATKIS, per 2 x 2 km grid cell, from which 6 SRs were defined (boxes).

Study regions (SR) were determined to be coherent and to contain grid cells from the upper ranks (>90th percentile) of the *CoOccInd*. SRs of a total area of >40,800 ha were identified to be investigated in high-resolution:

- For hops, two SRs in the Hallertau region were identified which is the world's largest coherent hop growing area (Wikipedia.org). 80% of the total hops cultivation in Germany is located in this region. The two selected SRs cover an area of >13,200 ha.
- A large fraction of apple cultivation in Germany occurs geographically highly distributed in low density (Figure 43). For apple cultivation six separate SRs were identified to be investigated in detail which cover an area of >27,600 ha. Five are located in the Lake Constance region and one in Saxony. The Lake Constance Region with its surroundings is one of the main apple cultivation regions in Germany.

6.1.4.4 High Resolution Data for Study Regions

The key objective was to develop geodatabases for the refined, landscape-scale exposure and effect assessment, containing all relevant LULC types in the selected SRs at appropriate level of detail. This demanded the manual digitising from target areas (hops/apple fields) and non-target areas (off-crop, *e.g.,* wood, meadow, herbaceous, shrubs) (Figure 44).

Figure 44: LULC types in hres (top: hres DOP; bottom: derived geodata).

Data were retrieved from high-resolution Digital Orthophotos (hres, DOPs) with a ground resolution of <0.5 m (Figure 44). The following LULC classes were derived from the high-resolution imagery (Figure 45): apple/hops cultivation, arable, herbaceous, shrubs, hedges, groves and bushes, meadow/grassland, meadow orchard, wood, water bodies (rivers, streams, lakes, ponds etc.), urban/transport infrastructure (residential, roads, farm tracks, railways etc.).

The digitised LULC data passed a quality check. A field observation, which was documented by georeferenced images, confirmed the results and identified further conservative definitions of the study: *e.g.*, in the geodatabase, apple cultivations are overly represented which led to an overestimation of exposure of off-crop from the use of PPP-1 in apple cultivations; hail-nets which presumably provide considerable sheltering against spray-drift were not considered in the exposure calculation; often rural roads occur between forest boundaries and cultivation which are typically not represented in the geodatabase, *i.e.*, in the geodatabase immediate adjacency is given; type 'herbaceous' often occurs between crop and rural roads.

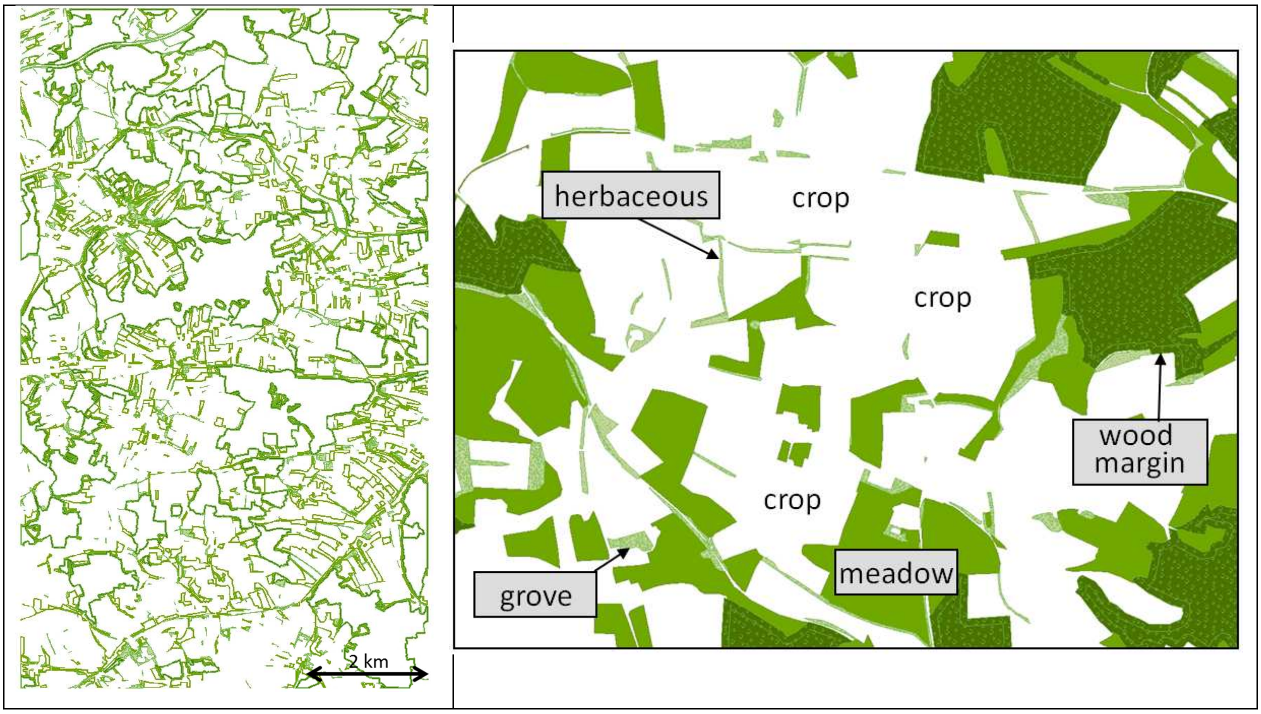


Figure 45: Illustration of off-crop as represented in the hres geodatabase (overview on one SR (left), detail (right)).

6.1.4.5 Landscape-scale Risk Assessment Using Xplicit

Off-crop areas were discretised into 3 m x 3 m segments (receptors). Spatiotemporally explicit calculations of exposure and effect (TER) of receptors due to spray-drift were performed using the Xplicit approach (Section 5.3).

Compared to the Tier-1 scenario the following factors were refined: landscape structure; variability of wind directions; variability of spray-drift deposition. Variability of spray-drift depositions was represented by PDFs provided by Strassemeyer & Golla (J. Strassemeyer, B Golla, Julius Kühn-Institut, 2008, pers. comm., Golla *et al.* 2011).

The individual exposure calculation steps were rather simple and straightforward: at a given time-step *t* fields were randomly chosen to be applied. For an application event, a wind direction was randomly selected. Spray-drift deposition to off-crop habitats downwind ('receptors') was calculated taking variability of spray-drift depositions into account. The resulting PECs of all receptors over all time-steps were recorded (→PEC(r,t) table). For N individual Monte Carlo trials this resulted in N PEC(r,t) tables. Evaluation of outcome: the maximum PEC of each receptor over the simulation time was calculated (for each of N PEC(r,t) tables). From the resulting distribution of the maximum PEC over all receptors of each Monte Carlo run, the 90th percentile PEC ('P90 PEC') was derived. From the resulting *N* P90 PEC, the expectancy value was derived (<P90 PEC>). As the entirety of all receptors were defined to represent a reasonably conservative set of off-crop habitats, this <P90 PEC> was considered to represent a realistic worst-case exposure value for off-crop.

Results were evaluated at different scales (regional, habitat patch, local habitat segment (receptor) scale). TERs and fraction of off-crop of TER < 5 were calculated, the spatial and temporal recovery potential of off-crop areas of TER < 5 was assessed, and the aggregation potential off-crop areas of TER < 5 was investigated.

6.1.4.6 Calculation of Recolonisation Distances

NTA populations effected by spray-drift deposition of a PPP are generally considered to have an internal and external potential to recover. A measure which depicts recovery potential from external sources is the recolonisation distance. Although a TER < 5 of an off-crop section does not necessarily indicate significant effects on population level, a TER < 5 was conservatively used to mark off-crop sections which need to be recolonised.

Recolonisation distance denotes the shortest distance of a receptor of TER < 5 (at least a single time step of the simulation) to the nearest receptor without TER violation (TER ≥ 5).

These distances were calculated by means of a geoprocessing service (*Xplicit-Distance*, Section 5.3.5.6), which was available through an ArcGIS Geoprocessing Service (running on ArcGIS Server, ESRI 2012). The service demanded a list of receptors with TER violation as input and provided the distance to the nearest receptor without TER violation. As recolonisation potential mostly occurred from within the same off-crop patch, taking barriers into account was not necessary and would have led to an overly complex approach.

For each study region three Monte Carlo runs were randomly chosen to be evaluated by *Xplicit-Distance*. The maximum recolonisation distances were reported (maximum of three medians and maximum of three 90th percentile distances).

In addition, recolonisation distances were exemplarily calculated by excluding, (i) recolonisation sources that showed a TER < 5 in a previous PPP-1 use season, and (ii) sources potentially of TER < 5 due to spray-drift depositions from PPP uses in arable crops. Results were compared to recolonisation distances obtained without this additional context.

6.1.4.7 Country-level Analysis

Although the site selection process was designed to assure the identification of SRs of high co-occurrence of crop and off-crop, and hence, assure conservatisms of results with respect to the entirety of cultivation conditions in Germany, the results obtained for the SRs were set in context to the country level.

To systematically explore landscape structure, metrics were used which indicated the potential of off-crop to be of TER < 5, aggregation of TER < 5 off-crop areas, and connectivity of off-crop. For 2 km x 2 km grids standard metrics of landscape ecology were employed (Table 19) to examine the spatial relations between crop, off-crop and 'TER < 5 off-crop' (FRAGSTATS, McGarigal & Marks 1995, McGarigal *et al.* 2002, Leitao *et al.* 2006) based on the German-wide topographical data ATKIS (BKG 2006).

6.1.5 Results and Discussion

Refined risk characterisation was conducted at three different scales: regional- (SRs), patch- (individual off-crop habitat, *e.g.*, herbaceous area), and receptor-scale (habitat segment). In addition, the country-scale (Germany) was addressed by setting the results obtained at regional scale in context via topographic data and landscape metrics.

6.1.5.1 Regional-Scale

The refined risk characterisation on regional-scale (SRs) shows that limited fractions of NTA habitats are expected to show TER violation (TER < 5, denoted as '<f_offCrop>'): <f_offCrop> = 3.5% for hops, <f_offCrop> = 6.8% for apple cultivations. Considering the 90th percentile (P90) as a realistic worst-case exposure value, TERs >> 5 result for both uses (hops, apple), which shows that to a large extent NTA habitats are unlikely to receive spray-drift entries leading to unacceptable risk. An example distribution of minimum TERs (over simulation period, '*minTER(r)*|time') obtained for off-crop receptors in an apple SR is shown in Figure 46.

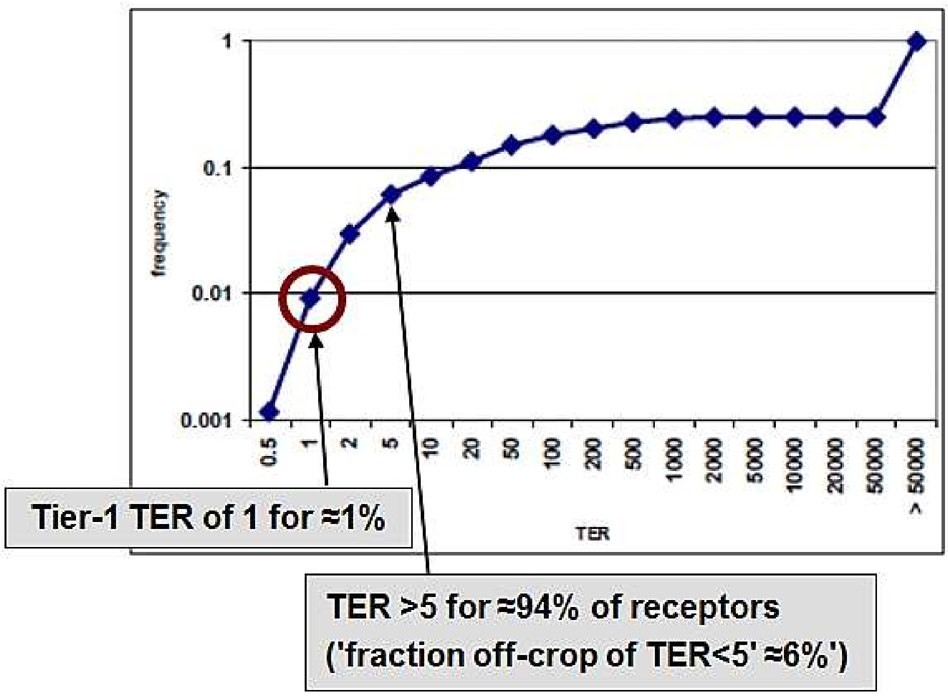


Figure 46: Exemplary cumulative frequency of *minTER(r)*|time (1 Monte Carlo run; 1 SR).

The distribution of fractions of NTA habitat segments of TER violation in a region (TER < 5, 'f_offCrop') can be illustrated as a risk curve (Equation 11, Figure 47). The risk curve shows, that, at regional scale, the fraction of NTA habitats of TER < 5 is expected to be approximately the same every spraying season of PPP-1 (around 7%). The patch/field scale is in-between the local and the regional scale. Therefore, although there is considerable variability in exposure at local (receptor) scale, at a higher hierarchical scale, this variability almost disappeared. Here, this is simply due to the fact that the variability in the direction-distance distribution between the fields and the NTA habitats become independent from direction, *i.e.*, the effect of wind variability is significantly reduced (Schad & Schulz 2011). In case the landscape structure shows preferences with directions this relationship is different. This phenomenon is proposed to be taken into account when investigating propagation of parameter uncertainty.

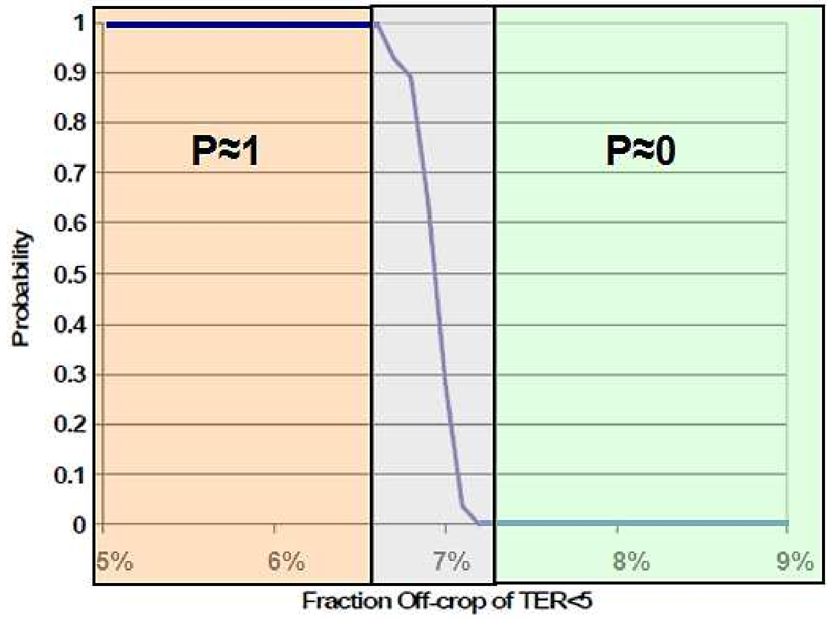


Figure 47: Risk curve of fraction of off-crop of TER < 5 (based on *minTER(r)|time*); the part of the curve in the grey area shows that, although processes are stochastic at local scale, at regional scale, only low variability of risk ('stable result') occurs.

$$P(f_{TERviolation} \geq f_{receptors}) = 1 - \int f(f_{TERviolation})\, df_{TERviolation}\ ,\ (0 \leq f_{TERviolation} \leq f_{receptors})$$

Equation 11

In order to further assess the spatial and temporal dimension of risk, so called recolonisation distances were calculated, providing information on 'how far a species might need to travel' to recolonise a habitat fraction that has received a TER < 5, and 'how long it takes' until such a habitat fraction can be recolonised (*i.e.*, TER increased to ≥ 5 due to dissipation of the a.s.).

The results show, median recolonisation distances are 4.2 m (90^{th} percentile (P90) recol.-dist. = 16.6 m) for hops, and 5.3 m for apple cultivations (P90 recol.-dist. = 21.2 m).

The entirety of results allow for the following summary on risk at landscape-scale:

i. NTA habitat fractions of TER < 5 are to a large extent well connected to habitat fractions of TER ≥ 5, which indicates a generally high recolonisation potential between potentially effected habitat fractions and refuges.

ii. Recolonisation can mostly occur from within the same NTA habitat that has partly received exposure leading to TER < 5, *i.e.,* refuges mostly exist in the same habitat.

iii. The findings in (i) and (ii) demonstrate that spatial aggregation of effects (TER < 5) is unlikely to occur.

For the characterisation of the temporal dimension of risk, temporal recolonisation 'distances' (in [days]) were assessed: For both crops, the median temporal recolonisation distance are about 6-7 days (P90 temporal recol.-dist. = 12.5 days for hops and 15.2 days for apple cultivations). These results show that the violation of the TER = 5 threshold (referring to reproduction effects of the most sensitive species) are temporally limited to about 1-2 weeks after PPP-1 has been used in all hops/apple fields.

Receptors with higher temporal recolonisation 'distances' apparently occur close to field boundaries where higher spray-drift deposition occurs. This obviously leads also to larger spatial recolonisation distances. This relationship between spatial and temporal recolonisation distances is exemplarily shown (for 1 SR) in Figure 48. As the graph demonstrates, this correlation is not particularly pronounced.

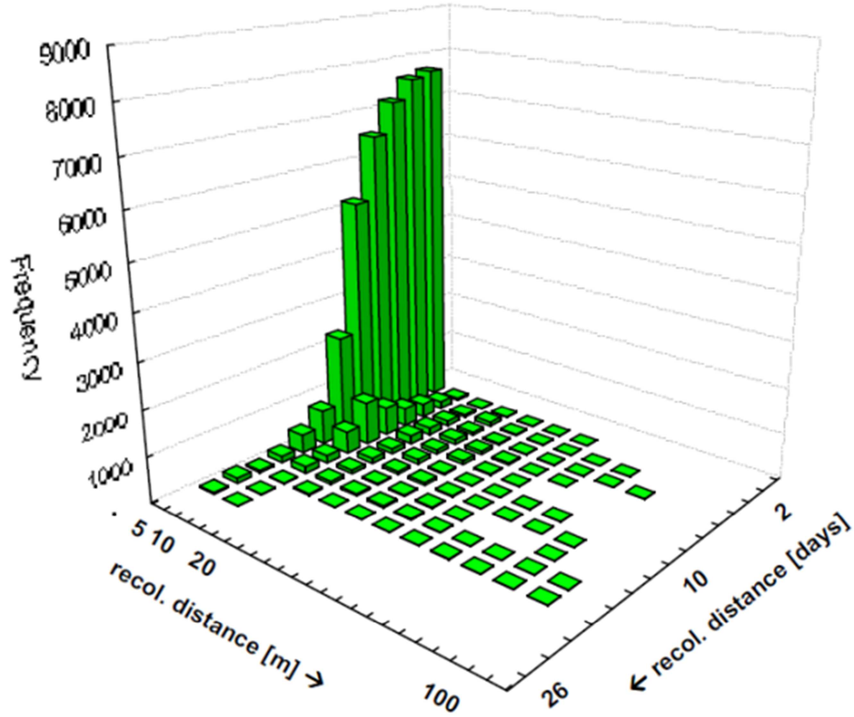


Figure 48: Illustration of relationship between spatial and temporal recolonisation distances.

Beside the distance between a receptor of TER < 5 and one of TER ≥ 5, the number of receptors (of TER < 5) which are recolonised by one single receptor (of TER ≥ 5) provides supporting information on the recovery potential, hence, for risk characterisation. An analysis showed that half of the receptors (of TER ≥ 5), which serve as recolonisation source, provide a source for only 1-3 receptors with TER violation.

In order to assess the very conservative assumption that population in off-crop areas of TER < 5 do not recover within one year, receptors of TER < 5 in a previous season were excluded from the recolonisation assessment. Resulting increase in recolonisation distances, which follows from reducing potential recolonisation sources, is of limited extent, as this 'effect-transfer' from over seasons does not lead to a significant change in the recolonisation potential present in the cultivated landscape, and hence, underlines the good connectivity of these.

A further evaluation of the recovery potential examined recolonisation distances when excluding receptors occurring in the vicinity of arable land and of TER < 5 in previous season. This simulates to conservative assumption that a PPP-1-like PPP is concurrently used on hops/apple and all arable fields in the SRs. The results show, that the increase in recolonisation distances which follows from excluding off-crop in the vicinity of arable land as recolonisation source is of insignificant effect. The main reason for this is the structure of land use/cover, as cultivation regions are dominated by hops or apple cultivations, as arable often directly borders on other land uses (than off-crop), and that off-crop areas of TER < 5 are generally well connected to such of TER > 5 in their immediate adjacency.

6.1.5.2 Patch-Scale

The patch-scale refers to the individual NTA habitat (*e.g.*, an herbaceous area, a hedgerow, a grove, a wood margin, etc.), *i.e.*, results were analysed for each individual habitat. In particular, the patch-scale allows to address questions revolving around potential aggregation of effects and generic RM (*e.g.*, landscape management).

Habitat types of highest potential risk were subject of patch-scale analysis. They were identified from results obtained at regional scale. Wood margins, grassland (meadow, pasture), meadow orchards, groves, hedges and related types show lowest risk, *i.e.*, highest levels of protection (numerically shown *e.g.*, in TER values >>5). For off-crop type 'herbaceous' the highest habitat fractions of TER < 5 were obtained. This is in agreement with intuitive expectation as the type herbaceous often occurs in direct vicinity of fields. For the risk characterisation of NTAs it has to be taken into account that herbaceous habitats account for <10% of NTA habitats in total, and that 'herbaceous' is mostly represented by comparably small areas often occurring as strips between fields and roads, and so, are typically affected by various anthropogenic impact (*e.g.*, fertiliser, maintenance).

As an example for patch-scale analysis, the fraction of TER violation (TER < 5) of each individual NTA habitat ('*f_offCrop*') was calculated. Exemplary results are shown in Figure 49. The frequency distribution shows *f_offCrop* subsequent to a spraying period (*i.e.*, results of a randomly selected Monte Carlo run of 1 SR). As the distribution demonstrates, about half of patches in the cultivated landscape are unaffected (53%). Towards higher fraction of TER < 5, the graph shows a clear tailing, *i.e.*, increasing *f_offCrop* occur in smaller number of off-crop patches. However, at the end of the distribution, about 7% of patches have 0.9-1.0 fraction of their area of TER < 5.

To characterise these 7%, the data were investigated by off-crop type (Figure 50). As the box-plot demonstrates, larger fractions of TER < 5 at patch-scale predominately occur for off-crop type herbaceous. In the total landscape, off-crop type herbaceous accounts for only 4% of off-crop. Further analysis steps to characterise herbaceous patches of high *f_offCrop* showed that such patches are mainly small herbaceous strips which occur between fields and rural roads (Figure 51), a land cover type that is generally subject to a range of land management impacts.

These characterisations provide new insights in potential risk of NTA across their habitats, and hence, a sound basis for RA and RM decisions.

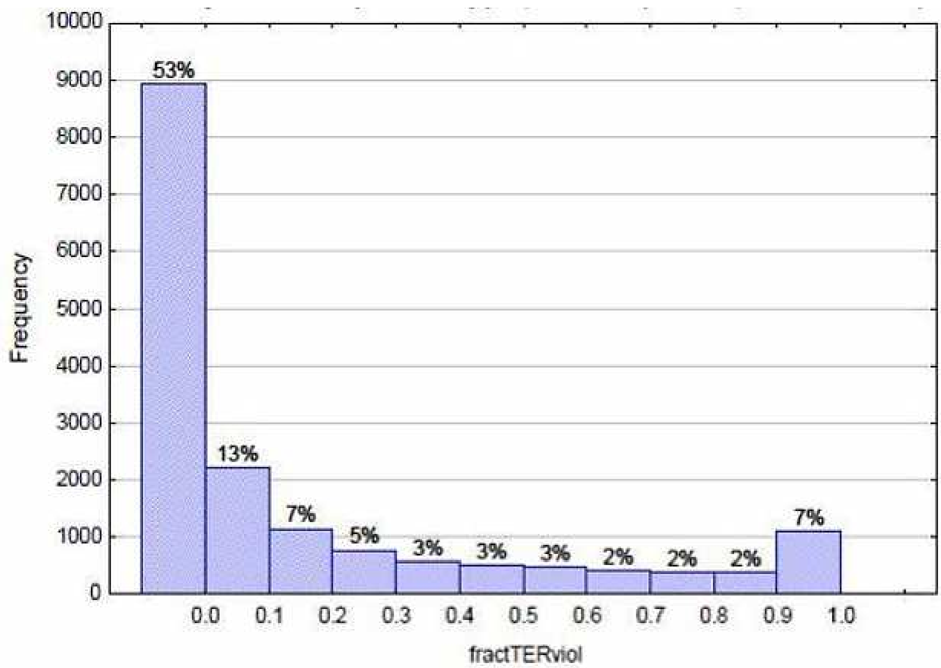


Figure 49: Fraction of off-crop patches of TER < 5 (based on *minTER(r)|*$_{time}$) (1 Monte Carlo run, 1 SR).

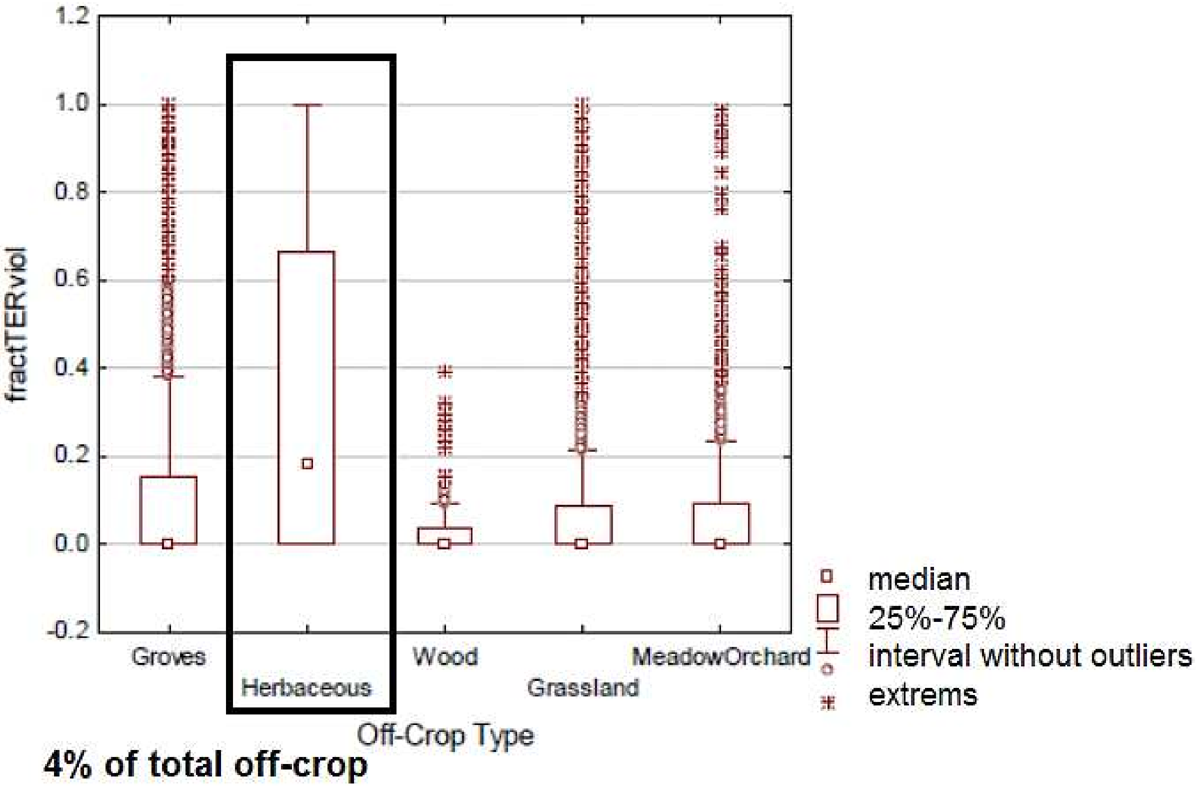


Figure 50: Fraction of off-crop patches of TER < 5 by off-crop type (based on *minTER(r)|*$_{time}$) (1 Monte Carlo run, 1 SR); type 'Herbaceous' highlighted by frame.

Figure 51: Example for type 'herbaceous' occurring in apple field vicinity.

6.1.5.3 Receptor scale

The receptor-scale refers to the smallest unit of analysis, the individual receptor that represents a small NTA habitat segment (3 x 3 m^2). At receptor-scale, questions with regard to potential risk, *e.g.*, of small local populations and their relationship to their surrounding can be investigated.

As an example assessment the probability of TER < 5 ($P_{(TER < 5)}$) of each individual receptor was calculated (frequency interpreted as probability) and analysed in terms of recurrence time. As the distribution of $P_{(TER < 5)}$ demonstrates, >80% of receptors are expected of TER < 5 every 10 years (or longer), <10% of receptors are of TER < 5 every other year, and only <1% of receptors are of TER < 5 every year.

The receptor-scale is the scale of highest variability of exposure and risk. As illustrated in the example analysis, risk characterisation at receptor-scale *e.g.*, supports assessments of potential long-term effects on local populations.

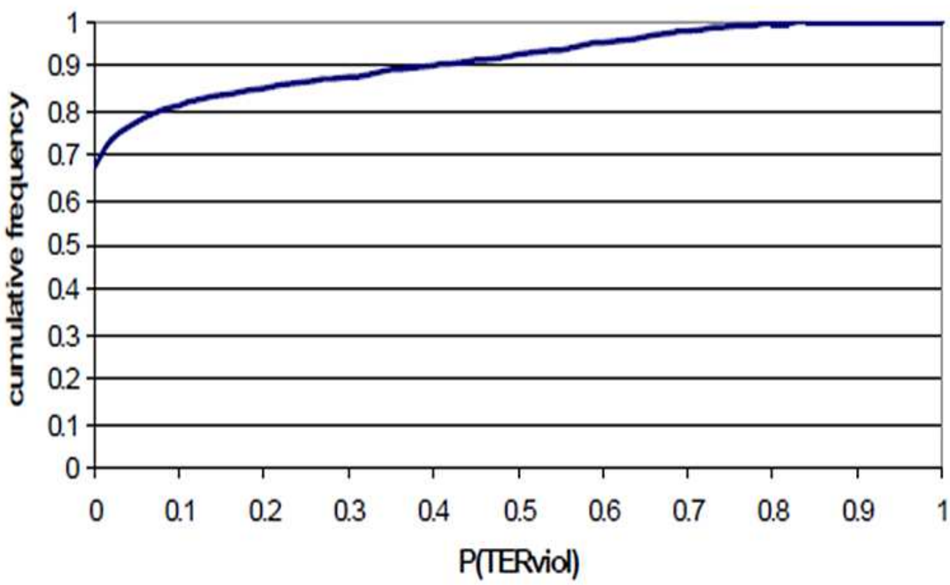


Figure 52: Cumulative frequency of $P_{(TER < 5)}$ of each individual receptor (based on *minTER(r)|time*), all Monte Carlo runs).

6.1.5.4 Transfer to Country Level

The findings of the detailed landscape-scale risk characterisation obtained for the SRs were set in context to the country level by means of landscape metrics (Section 6.1.4.7), using the German-wide topographic geodata ATKIS. Landscape metrics were calculated for each 2 km x 2 km grid which includes apple/hops cultivation.

Risk characterisation aspects of the analysis were (i) potential of off-crop to receive significant spray-drift deposition leading to TER < 5, (ii) aggregation potential off-crop areas of TER < 5, and (iii) off-crop connectivity / recolonisation potential.

<u>Summary of results:</u>

The results of the transfer analysis to country level consistently supported the conservative character of the SRs, hence, emphasised the protective character of the study results and conclusions drawn for the SRs. It was shown for both crops that,

i. for the majority of cultivations in Germany outside the SRs the potential of off-crop to receive significant spray-drift from the use of PPP-1, leading to TER < 5, is in the main lower than for the SRs,

ii. off-crop areas of TER < 5 occur distributed in the landscape and are mostly interspersed by or connected to off-crop of TER > 5, hence, aggregation is unlikely to occur,

iii. due to the size and extent of off-crop patches and their connectivity, as well as the interspersion of areas of TER < 5 and TER > 5, the potential for recolonisation is generally high.

A summary on the metrics used in the context-setting process is provided in Table 19 (abbreviations: FRAGSTATS, McGarigal & Marks 1995, McGarigal *et al.* 2002, Leitao *et al.* 2006).

Table 19: SRs in context to Germany-wide cultivation conditions - evaluation summary.

Evaluation Target	**Key Metric**	**Evaluation**
potential of off-crop to be affected (*fractTERviol*)	CoOccInd $A_{offCrop}$ / A_{crop} CONTAG ECON	all indices consistently shown that the SRs are conservative; therefore, for the majority of cultivations in Germany lower risk for NTA expected than obtained in the SRs (lower PEC, higher TER, lower *fractTERviol*)
aggregation (patch-, landscape-, country level)	ENN PROX TER>/< 5 distance GYRATE AREA (_MN, _SD) (visual inspection)	at patch-level, the sizes and elongations of patches show that larger fractions of individual patches of TER < 5 (high *fractTERviol*) are not to be expected frequently; patch fractions of TER-violation mostly border on areas of TER > 5, *i.e.*, high interspersion of 'TER</>5 areas' at landscape-scale, aggregation of TER-violations is physically limited to the co-occurrence pattern of crop and off-crop (and the variabilities driving exposure); an estimated worst-case pattern of TER-violations ('$A_{TERviol}$') showed considerable spacing with high variability and, as obtained for the patch-level, will be highly interspersed with patches of TER > 5; results are supported by visual inspection
recolonisation, connectivity	GYRATE AREA (_MN, _SD) TER>/< 5 distance $A_{offCrop}$ / A_{crop} (visual inspection)	patch sizes, elongations and total off-crop present demonstrate high connectivity and recolonisation potential at landscape-scale; at patch-level, low TER>/< 5 area distances demonstrate that recolonisation can mostly happen from within an individual patch

As an example, a simple metric to assess the potential of off-crop to receive significant spray-drift depositions from cropped areas (high *fractTERviol*) is shown below.

On the hypothesis that the higher the ratio of off-crop area by crop area per grid ($A_{offCrop}$ / A_{crop}) the higher the likelihood that off-crop occurs far from crop ('saturation effect of co-occurrence'), *i.e.*, as a trend, high '$A_{offCrop}$ / A_{crop}' correspond to low *fractTERviol* and lower *fractTERviol* variability.

($A_{offCrop}$ / A_{crop}) was calculated per 2 km x 2 km grid (ATKIS). For landscapes of low fraction of off-crop ($A_{offCrop}$ / A_{crop} << 1), *fractTERviol* can be quite variable due to sensitivity to the co-occurrence with crop.

The relationship between the ratio of off-crop area by crop area ($A_{offCrop}$ / A_{crop}) and *fractTERviol* is shown in Figure 53 for the SRs. The trend of lower *fractTERviol* with higher ($A_{offCrop}$ / A_{crop}) is confirmed for the SRs.

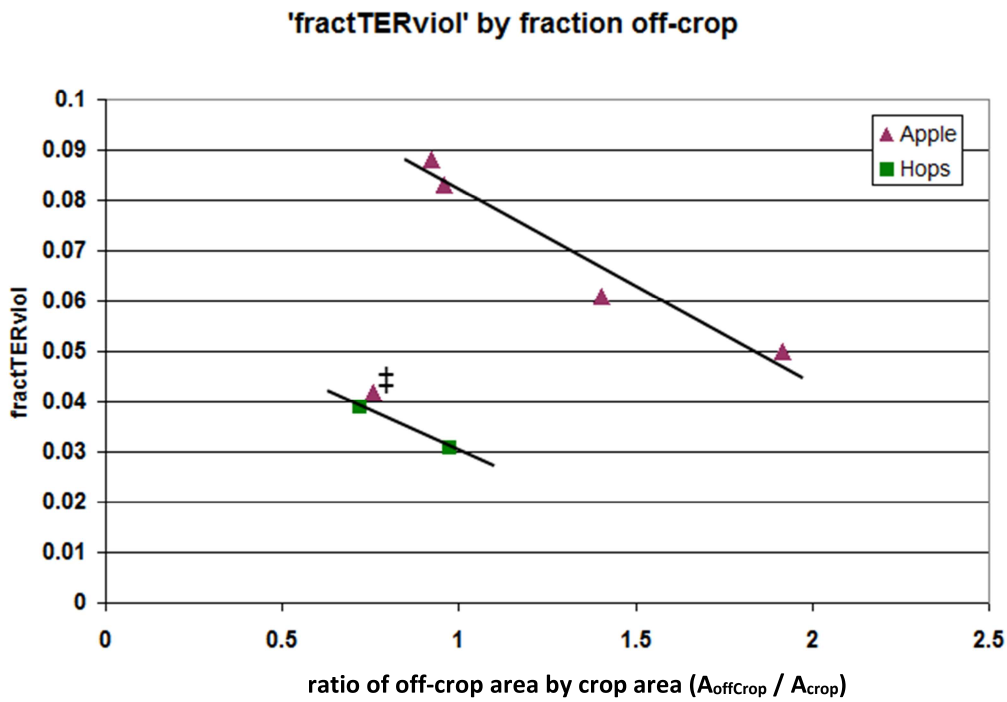


Figure 53: Relationship between the ratio of off-crop area by crop area ($A_{offCrop}$ / A_{crop}) and *fractTERviol* for the SRs (‡ data of most intensive cultivation, Saxony).

The ratio of off-crop area by crop area ($A_{offCrop}$ / A_{crop}) was calculated for all 2 km x 2 km grids containing hops/apple cultivations across Germany (ATKIS). The results demonstrate (Figure 54) that >92% of grids containing apple cultivations (N_{grids} = 6,914) have a ($A_{offCrop}$ / A_{crop}) > 1 (Figure 53). Thus, this relationship indicates that high *fractTERviol* are unlikely to frequently occur outside the SRs.

This simple metric and the more sophisticated metrics on landscape composition and structure (Table 19) consistently indicate that the refined landscape-scale risk characterisation for NTA was conducted in SRs representing conservative scenarios for NTA exposure due to spray-drift of PPP-1 also at country scale.

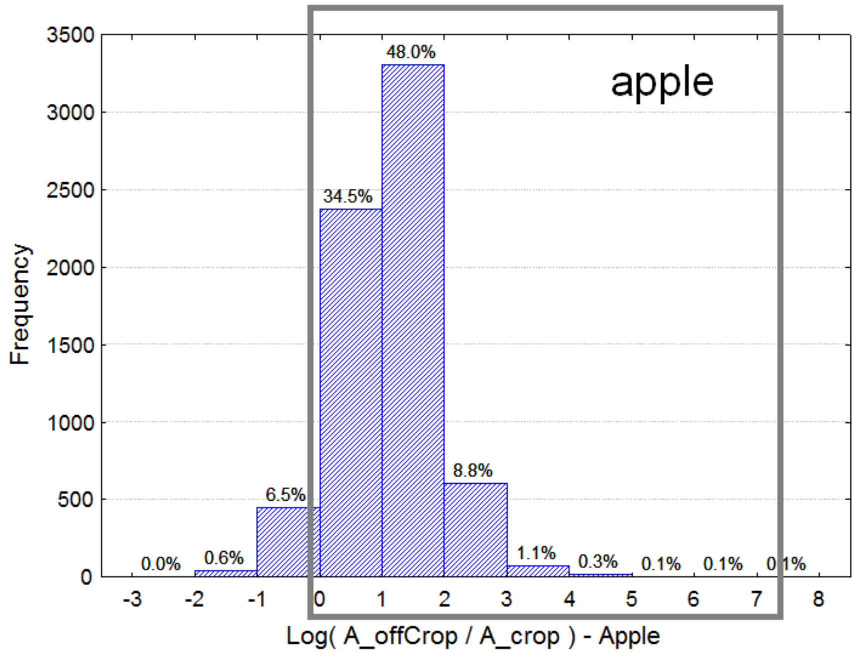


Figure 54: Ratio of off-crop area by crop area ($A_{offCrop}$ / A_{crop}) calculated for all 2 km x 2 km grids containing apple cultivations across Germany; the box highlights the fact that >92% of grids (N_{grids} = 6,914) show ($A_{offCrop}$ / A_{crop}) > 1.

6.1.6 Conclusions

The risk characterisation for the conservative SRs shows that for both crops, TERs above the trigger value of 5 are obtained at landscape-scale. Fractions of NTA habitats of TER < 5 are <10%. The spatiotemporally explicit analysis of the recolonisation potential shows that fractions of habitats of TER < 5 are well connected to such of TER > 5 and that the duration of TER < 5 is typically about a week. At the landscape-scale, as well as the scale of the individual habitat patch, aggregation of areas of TER < 5 is not likely occur, due to general interspersal of areas of TER < 5 with such of TER > 5.

The results of the transfer analysis to country level consistently support the conservative character of the SRs, hence, emphasise the protective character of the study results and the conclusions drawn for the SRs. It was shown for both crops that, for the majority of cultivations in Germany outside the SRs the potential of off-crop being affected is lower than for the SRs.

In summary, the results show that the risk characterisation of Non-Target-Arthropods can be significantly improved, compared to the knowledge on real-world risk at Tier-1 RA level, by assessing the exposure and effect potential due to spray-drift at landscape-scale. The refined RA is mainly a result of the real-world spatial relationship between the hops and apple cultivations and off-crop, the composition and configuration of land use/cover and the variability of local spray-drift depositions. Together, these 'landscape factors' can be regarded as representing naturally present mitigation. Under more realistic conditions the spatial and temporal extent of TER violation (TER < 5) is limited. Correspondingly the occurrence of the conditions of the Tier-1 scenario of spray-drift exposure is likewise limited.

For the use of PPP-1, protection level can presumably be further increased using a 5 m in-crop buffer as an additional RM measures which was not taken into account in the analysis. Beyond the RA for PPP-1, the landscape-scale results can also support generic RM (*e.g.*, landscape management).

6.1.7 Outlook

According to forthcoming SPGs (EFSA 2010a, EFSA 2010b), for protection of NTAs, the focus *Biological Entity* is the (meta-) population. Protection goal *Attributes* are *e.g.*, abundance or population recovery (at appropriate spatiotemporal scales). Therefore, linking a (meta-) population model to Xplicit is a proposed next step, in order to propagate spatiotemporally explicit exposure and individual effects (*e.g.*, clutch size reduction) to the (meta-) population level. A potentially appropriate (meta-) population model for NTAs was presented by P Thorbeck at SETAC Europe 2011 (SETAC 2011) using an *Individual-Based-Model* approach which is currently discussed (MODELINK, SETAC Europe Technical Workshop, October 2012 and April 2013).

Studies as the presented can make a contribution to the development of Reference Scenarios in the context of SPGs (EFSA 2010a, EFSA 2010b).

Exposure of NTAs is driven by spray-drift depositions in 3-dimensional vegetation structures. An improvement of the currently available empirical data on spray-drift depositions (Rautmann *et al.* 2001) towards real-world structures is needed to further increase realism in landscape-scale exposure and effect assessment.

Reduction of variability over (hierarchical) scales, as shown in the present study, suggests that similar reduction applies to the propagation of parameter uncertainty. This can affect the characterisation of the degree of certainty in simulation outcome, RA and RM decision-making. This phenomenon needs a systematical investigation, which can be supported using the *Xplicit-Framework* for the propagation of uncertainties in systems of hierarchical scales ('UASA', Section 4.5.4 and 5.3.4.13).

6.2 Risk Characterisation for Non-Target-Terrestrial Plants

At Tier-1 RA level of NTTPs, comparably broad data on individual-level ecotoxicological effects are generated, of which only limited use in made in RA. The case study presents the use of the Xplicit approach in a first step to propagate variability of individual-level effects and of exposure to the plant community level, considering distinct risk dimensions.

6.2.1 Lessons Learned

- The Xplicit approach provides a means to raise NTTP RA from the protective lower Tier-1 level towards a RA level that corresponds to actual NTTP protection goals (EFSA 2010a, 2010b, Section 4.3.2.1) and that allows to quantify risk of NTTPs.
- The adaptability of the *Xplicit-Framework* has led to an *Xplicit-NTTP-Model* which is capable to assess different risk dimensions (*species*, *Assessment Endpoint* (*AE*), *space*, *(time)*). The *Xplicit-NTTP-Model* calculated spatiotemporally explicit effects using dose-responses of 10 species and 7 attributes (70 *species-AEs*).
- The *Xplicit-NTTP-Model* can be used at different scales. In this case study the edge-of-the-field- and the regional-scale were assessed. First scenarios for refined NTTP risk characterisation were illustrated. This demonstrates that the approach can make a valuable contribution at different complexity levels to future scenario development (Reference Scenarios, EFSA 2010a).
- *Xplicit-Models*, like the *Xplicit-NTTP-Model*, allow to stepwise introduce context into RA (from *AutContext* to *SynContext*, Section 4.1) in order to assess the range of relevant risk driving factors, including, *e.g.*, landscape management. In this respect, the use of an *Individual-Based-Model* for plant communities is planned, which should allow to assess individual-level effects at community level in context of competition, agricultural and environmental factors (introduced stepwise).

6.2.2 Abstract

Natural or semi-natural plant communities (Non-Target-Terrestrial Plants, NTTP) occurring in cultivated landscapes meet particular environmental conditions. Depending on cultivation density plant community habitats are often limited to *e.g.*, herbaceous stripes and patches, hedges, riparian vegetation, groves, or wood margins. Agriculturally managed grassland and meadows provide a further type of plant communities. As part of the cultivated landscape all these plant communities are managed and affected by a number of conditions, *e.g.*, habitat sizes, connectivity/isolation, fertiliser, maintenance, mechanical effects, herbicidal effects etc.

This case study is part of a project which is intended to take initial steps towards introducing more context into NTTP RA. In the first step of the project (the present case study), variability of ecotoxicological effect data on individual-level and exposure refines risk characterisation. The second step of the project will propagate these individual-level effects to plant population and community level, which are the actual biological entities of RA and RM (EFSA 2010a, 2010b, Section 4.3.2), by means of *Individual-Based-Modelling*. This will already include aspects of the

third step, which is proposed to take the view of the ecosystem of plant communities and their agricultural and environment conditions (*SynContext*, Section 4.2).

Current Tier-1 RA of NTTPs is protective, and so, does not allow for risk quantification. The present case study (1st step of the full project outlined above) started at the definitions and data at Tier-1 RA level for spray-drift, which was not passed by the test herbicide. An *Xplicit-NTTP-Model* was derived from the *Xplicit-Framework* and was used to refine risk characterisation by taking into account variability of exposure and individual-level effects (dose-responses of 10 species and 7 attributes). Quantification of effect extent was done for the three risk dimensions *species*, *Assessment Endpoint* (*AE*) and *space*, at edge-of-the-field- and regional-scale. Exposure calculation considered variability of wind directions and of spray-drift depositions (PDFs of Golla *et al.* 2011). As the case study design was developed on the basis of the Tier-1 scenario and carries characteristics of this RA level, results are considered immediately applicable to refine regulatory RA of NTTPs.

At the edge-of-the-field-scale, a small NTTP community of 3 m width occurring downwind from the field was assessed. Only a small fraction of the 70 endpoints (10 *species*, 7 *AEs*) of the plant community showed pronounced effects, among which sublethal were dominating: *e.g.*, at the 90th percentile of the spatial community extent, 2 *species-AEs* showed ≈0.3 effect level (30%), both of which were sublethal. A single survival effect of 0.1<effect<0.2 was observed. In total, 6 of the 70 *species-AEs* showed effects of 0.1<effect<0.4. At 50th percentile, a single *species-AE* showed effects of 0.2<effect<0.3 (sublethal). A single survival effect of 0.1<effect<0.2 was observed. In total, 3 of the 70 *species-AE* showed effects of 0.1<effect<0.3 (sublethal).

At regional scale, a test landscape of dense arable cultivation was investigated. Only herbaceous NTTP communities were assessed, which is conservative as this type frequently occurs in close vicinity to fields and is typically of small spatial extent, compared to, *e.g.*, meadows. Four different NTTP community sizes were assessed, starting at 1 m from field edge, and extending up to maximum distances of 3 m, 10 m, 50 m and 100 m. Parts of the plant communities were found of same risk as at edge-of-the-field-scale. This is apparent, as always parts of such plant communities occur immediate to the field boundary. The influence of variability of conditions at regional-scale is shown by the 50th percentile effects, which are significantly lower than at edge-of-the-field scale. Thus, the regional-scale analysis demonstrates that even for small herbaceous plant communities occurring in immediate vicinity to fields in dense cultivations, natural variability of exposure conditions and landscape structure affects risk characterisation. Regional scale analysis also emphasises the importance of habitat size, and hence, of landscape management (*e.g.*, structure) for plant communities.

As only a small fraction of the plant community showed pronounced effects, the result encouraged the question of whether sublethal effects on individual-level which are limited in effect extent, to a fraction of species, Assessment Endpoints, and spatial extent can cause unacceptable effects at community level under real-world conditions. These results of the present case study will be used in the second step of the project: An approach towards risk characterisation at plant population and community level was outlined and an *Individual-Based-Model* was identified (May *et al.* 2009) to propagate the obtained individual-level effects over *species*, *Assessment Endpoint* (*AE*) and *space* to the community level. This will also allow to further specify risk characterisation for biodiversity protection goals (EFSA 2010a, 2010b, Section 4.3), and hence, to take an ecosystem viewpoint of the plant communities (third step).

6.2.3 Introduction & Objectives

Natural or semi-natural plant communities occurring in cultivated landscapes meet specific environmental conditions. Depending on cultivation density (land use), habitats of plant communities are typically limited in size and type(herbaceous patches, hedges, riparian vegetation, groves, or wood margins). Managed grassland and meadows provide a specific type of plant communities as they are directly managed with agricultural purposes. Management of agricultural landscapes affects (semi-) natural plant communities either by direct measures (*e.g.*, land use, landscape planning, maintenance of riparian vegetation, cutting of herbaceous field strips) or indirectly, *e.g.*, by nutrient input or mechanical effects. Fallow lands represent a further type of semi-natural plant communities, yet, their occurrence depends on regulatory and agricultural conditions which can be subject to short-term changes. Biodiversity goals (Section 4.3.3) requesting for larger fractions of (semi-) natural land on the one hand, and requests for agricultural products on the other hand are counteracting forces for the occurrence of semi-natural plant communities. Human activities in cultivated landscapes cause dynamic conditions of (semi-) natural plant communities, first of all regarding cropping conditions including weed management using PPPs (herbicides). Spray application of herbicides on fields potentially involves a fraction of the sprayed amount drifting from the field and depositing in the vicinity. In RA and RM context, (semi-) natural plant communities which are not targeted by plant protection measures are referred to as Non-Target-Terrestrial Plants (NTTPs).

Risk of NTTPs to be adversely affected by spray-drift of PPPs is supposed to be largely driven by spatial and temporal variability of environmental, ecological and agricultural conditions. This variability results from, *e.g.,* the composition and structure of landscapes, stochasticity of application or weather events, spray-drift variability, species occurrence, species sensitivity and life cycle trait, plant community composition, and application technology.

Current EU legislation (EC 2009a) provides general protection goals for NTTPs, *e.g.,* "*no decrease in biodiversity*" (Section 4.3.2). Protection goals have not been specifically defined yet, *e.g.,* EFSA states (EFSA 2010a): "*General protection goals are stated in European legislation but specific protection goals (SPGs) are not precisely defined. These are however crucial for designing appropriate RA schemes.*". EFSA proposes options to define SPGs (EFSA 2010a, Section 4.3.2 and 4.3.3). SPGs will likely require a more explicit assessment of the spatial and temporal extent of risk, taking different scales into account. For NTTPs, SPGs are likely to focus on the biological entities *population* and *community* (Section 6.2.3.1).

The standard ecotoxicological effect assessment of NTTPs focuses on the biological entity *Individual*, testing different attributes (*e.g.,* laboratory tests on vegetative vigour, survival, seedling emergence) for a number of species. Variability of effects are observed over individuals. PPP exposure rates [g a.s./ha] are derived at which x% of the individuals are effected (ERx). The standard Tier-1 RA does not make use of this range of data, but derives only the lowest effect rate [g a.s./ha] from all species and AEs tested. The next level in the tiered RA scheme makes more use of the available data by using the ERx (or NOECs) from all tested species in Species Sensitivity Distributions (SSD). From the SSD, a low percentile is taken as the 'Hazard Concentration' at which x% of the species are affected (*e.g.,* HC5 approach). Again, the lowest HC5 value is used in the RA.

Similarly, in Tier-1 RA the exposure scenario for spray-drift is a conceptual simple point estimate of conservative characteristic. Spray-drift is regarded a major exposure route to NTTP communities as considerable fractions of the amount of PPP applied can drift across the field boundary and deposit in the vicinity. Spray-drift deposition was measured in a number of field trials (Ganzelmeier *et al.* 1995, Rautmann *et al.* 2001) which were evaluated to derive 90th percentile depositions for different distances from the field. These deterministic values build the basis of the standard exposure scenarios for spray-drift ('Tier-1' scenario) as part of the ecological RA in the European Union and its Member States (FOCUS 2001).

In essence, the Tier-1 RA scenario is of protective nature and relates conservative exposure to conservative effect assessment (Figure 55). In case the Toxicity-Exposure-Ratio (TER, including an Assessment Factor (AF) to account for uncertainty in species sensitivity) exceeds a predefined threshold acceptable risk is indicated. Not passing the Tier-1 assessment level says that the Tier 1 protection level is not reached, which does not indicate unacceptable risk, but indicates a requirement to refine the RA. Ultimately, risk acceptability has to be assessed in the framework of the protection goals.

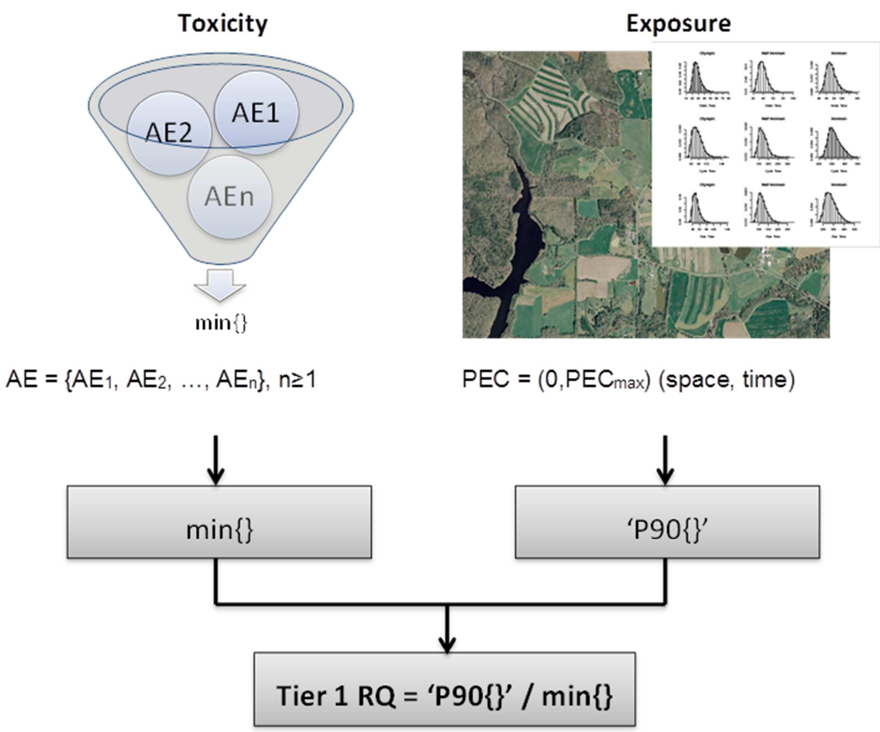


Figure 55: Illustration of Tier-1 RA approach (deterministic, RQ = Risk Quotient = TER^{-1}).

Ecological risk characterisation at landscape-scale constitutes a substantial step towards closing the gap between RA procedure and protection goals. At landscape-scale, the spatiotemporally extent of risk can be assessed on the basis of real-world (geo) data on land use, habitats and their connectivity, with focus on biological entities and attribute defined in protection goals.

Key objective of the present landscape-scale study was to take a stepwise approach towards refined risk characterisation for NTTPs in the context of SPG (EFSA 2010a, Section 4.3.2). The following refinements are taken into account:

- Full ecotoxicological effect data on species and Assessment Endpoints available at Tier-1.
- Natural variability of exposure due to spray-drift at different scales.
- Edge-of-the-field- and landscape-scale.
- Risk extent in different dimensions (*e.g.*, *species, AE, spatial*).
- Steps to propagate *Individual*-level effects to population- and community-level by means of *Individual-Based-Modelling*. Particular attention should be spend on plant competition (*e.g.*, probability of species to get out-competed). This has to be assessed specifically from the perspective of protection goals related to biodiversity.

Results should lay a foundation stone towards higher-tier RA for PPPs ("*Calibrating Tier-1*"). Results can also support the definitions of future SPGs for NTTPs and the development of corresponding scenarios (Reference Scenarios, EFSA 2010a).

The study can also contribute to develop adequate risk communication approaches in multidimensional risk characterisation and serve as basis for clear RM decision-making.

6.2.3.1 Protection Goals of Non-Target-Terrestrial Plants

Current EU legislation (EC 2009a) provides general protection goals, *e.g.*, "*no decrease in biodiversity*". Specific Protection Goals (SPGs) for NTTPs are envisaged (EFSA 2010a, EFSA workshop 2010b, EFSA Working Group on Terrestrial Plants working on a new Guidance Document, to replace EC 2002b).

SPGs are considered a prerequisite to adequate risk characterisation as a basis for RA and RM. SPGs are anticipated to define protection goals in different risk dimensions (EFSA 2010a), *e.g.*, *Biological Entity*, *Attribute*, *Magnitude*, *Spatial* and *Temporal Scale*, as well as degree of *Certainty*.

Although, final SPGs for NTTPs have not become available yet, some aspects can be anticipated from the available information (Figure 56, showing considerations from the EFSA workshop (ESFA 2010b). Here, the following aspects are of particular relevance:

- The (meta-) population/community level is the key *Biological Entity*.
- The occurrence of species and their abundance (resp. 'biodiversity'), *i.e.*, in simple terms the plant communities, are the targeted *Attributes.*
- Protection *Spatial Scales* range from edge-of-the-field to landscape. (Nature preservation areas are of particular importance, hence, protection level.)

Legal requirement	Specific protection goal	Ecological entity	Attribute	Scale			
				Magnitude of impact	Spatial scale of impact	Temporal scale of impact	
						Duration	Frequency
No decrease in biodiversity	No decline in biodiversity in the watershed / landscape	Meta-population to community					
			Species richness / biomass / abundance /	Small to medium effects	field	Days to weeks (max 4 to 6)*	See ELINK
			Biodiversity	Negligible effects in protected area and landscape / watershed	Landscape / watershed	Not relevant	Not relevant

Figure 56: Excerpt of SPGs for NTTPs discussed in an EFSA workshop (EFSA 2010b).

From these definitions one can preliminary conclude that,

- local and transitional effects to few species are acceptable,
- and that an approach (concept, data and tools) is necessary to quantify effect extent in risk dimensions.

Further important questions towards refined risk characterisation and ultimately, RM decisions (*e.g.*, buffer zones), concern the characterisation of *habitat type* and their SPGs, *i.e.*, "*which SPG (hence, protection level) for which habitat type?* Presumably, plant communities of higher protection level should have a minimum extent and/or should be of particular ecological importance, and should not be significantly affected by other factors (*e.g.*, fertiliser input, mechanical effects, mowing, etc.). The latter is the case for *e.g.*, small field margins of about 1 m width. Nature preservation areas are of particular importance, hence, of high protection level.

6.2.3.2 Risk Characterisation for Non-Target-Terrestrial Plants

SPGs provide the framework for risk characterisation (and communication) in terms of explicitly defining risk dimensions and assigning specific endpoints to these (*e.g.*, "*population*" as *biological entity*). Specific definitions are not yet available. Also, SPGs do not determine *how* to do related risk characterisation. Therefore, based on the currently available data and information a preliminary approach (concept, data + tools) has been developed and has been transferred in a corresponding project, which aims at refining the risk characterisation for NTTPs.

In the present case study (representing the first step of the full project), variability of ecotoxicological effect data on individual-level and exposure refines risk characterisation. Effect extent is quantified in risk dimensions (Section 6.2.3.1). The regional-scale plays an important role as risk of plant community refers to the spatial extent of effects. At regional-scale, exposure and effects of plant communities are driven by a number of factors, *e.g.*, landscape composition (land use/cover, type of plant communities), landscape structure (landscape configuration), variability of weather conditions and herbicide application, etc. The second step of the full project will propagate individual-level effects to plant population and community, which are the actual biological entities of RA and RM (EFSA 2010a, 2010b, Section 4.3.2), by means of *Individual-Based-Modelling*. This will already include aspects of the third step, which is proposed to take the view of the ecosystem of plant communities and their agricultural and environment conditions (*SynContext*, Section 4.1). (Ecological Modelling, Section 6.2.4.6).

6.2.4 Data & Methods

6.2.4.1 Plant Protection Product

A herbicide, with a broad dicot weed spectrum, was assessed, with a (normalised) application rate of 100 g a.s./ha (‘Herbicide-1’). A single application to arable crops was assessed (post-emergence). Application timing was not a relevant parameter with respect to the status of the study presented herein, as predefined conditions of the Tier-1 RA level were kept, *e.g.*, regarding the relationship between NTTP development stage and PPP use timing. The use of 90% spray-drift reducing application technology was assumed.

Effect data were taken from a 'Vegetative Vigour (VV)' and a 'Seedling Emergence (SE)' study (A Solga, BCS, pers. comm. 2011, unpublished data), which provided data for ten species, for each of which seven Assessment Endpoints were tested (emergence (SE), survival (SE, VV), dry weight (SE, VV), shoot length (SE, VV)). Dose-response curves (log-logistic) were calculated for 70 *species-AEs* from the data using the R-Statistics 'DRC-package' (CRAN 2012).

At regional-scale, exposure of local NTTP communities can potentially result from all surrounding fields, *i.e.*, can overlay. As a conservative assumption, dissipation of the substance on plant leaves was not taken into account (a DT50 = 9999 days was used), *i.e.*, effectively, spray-drift depositions from different fields could locally add-up.

6.2.4.2 Tier-1 Risk Assessment

The standard Tier-1 RA for NTTPs due to spray-drift essentially compares relative extremes in a TER (Toxicity Exposure Ratio) approach (at '*Deterministic*'-level): A minimum Assessment Endpoint (*AE*) is divided by a 'tail-end' exposure (90^{th} percentile PEC, Rautmann *et al.* 2001) (Figure 55). Acceptable risk is indicated in case TER > Assessment Factor (*e.g.*, AF = 5), which basically accounts for uncertainty in species sensitivity.

For the assessed use of Herbicide-1 a TER < 5 was obtained at Tier-1 ('*Deterministic*'-) level, *i.e.*, acceptable risk could not be demonstrated.

The Tier-1 RA level considers a refinement step referred to as *'Probabilistic'*-level. Probabilistic methods make use of species sensitivity distributions (SSD) in case data for a sufficient number of species are available. At *'Probabilistic'*-level, a HC5 approach is used (HC5: Hazard Concentration at which 5% of species in a specified (eco)system are assumed to be effected). The minimum HC5 over Assessment Endpoints is combined with the 90^{th} percentile exposure (same as at '*Deterministic*'-level). Again, an AF is imposed to account for species sensitivity uncertainty. The assessed use of herbicide-1 also fails the *'Probabilistic'*-level.

The Tier-1 RA level includes the following conservative assumptions regarding exposure:

- All NTTP communities occur in a distance of 1 m from arable fields.
- All NTTP communities occur downwind.
- 90th percentile spray-drift deposition (Rautmann *et al.* 2001).
- Considerable wind speed (Rautmann *et al.* 2001).
- Worst-case spray-drift deposits on plant surfaces (no filtering due to 3-dimensional vegetation structure).
- No spray-drift filtering by intervening vegetation, *i.e.*, full exposure of entire community.

On Tier-1 exposure conditions, downwind spray-drift depositions at 1 m distance are at 90th percentile about 1/360th and on average <1/700th (≈0.14%) of the field use rate (Rautmann *et al.* 2001, Golla *et al.* 2011). This ratio provokes the question whether a herbicide that is used at sensible rates to efficiently control weeds in the field can lead to significant damage to NTTPs from the perspective of actual NTTP protection goals which refer to the biological entities population and community (Section 6.2.3, 4.3). Thus, the efficiency of the Tier-1 approach regarding identification of risk acceptability of NTTPs is proposed to be examined.

6.2.4.3 Landscape-scale Risk Characterisation Approach

A stepwise approach was defined towards refined risk characterisation for NTTPs:

i. Step-1: Characterisation of *Individual*-level effects at different landscape-scales using spatiotemporally explicit exposure and effect assessment (Xplicit).
ii. Step-2: Propagation of refined *Individual*-level risk characterisation to population and community level by means of combining Step-1 results (Xplicit) to plant population and community models. This will already include aspects of the third step, which is proposed to take the view of the ecosystem of plant communities and their agricultural and environment conditions (*SynContext*, Section 4.2).

The present case study represents Step-1 of the analysis. For Step-2, a plant population and community model has been identified and discussed (May *et al.* 2009, Prof. F Jeltsch, University Potsdam, pers. comm., 2012).

In Step-1, the landscape-scale risk characterisation for NTTP included the following refinements compared to the Tier-1 RA level (Figure 57):

- Use of 70 dose-response relationships based on testing of 10 species and 7 *AEs* each.
- Spatiotemporally explicit exposure and effect assessment using an *Xplicit-NTTP-Model* (Section 6.2.4.5).
- Variability of spray-drift depositions at edge-of-the-field and regional-scale.
- At regional-scale, landscape composition and structure are taken into account, affecting the local crop-to-NTTP distance in different potential wind directions.
- Assessment of risk extent in different dimensions (*e.g., species, AE, spatial*) at edge-of-the-field and regional-scale. Risk characterisation for different plant community sizes.

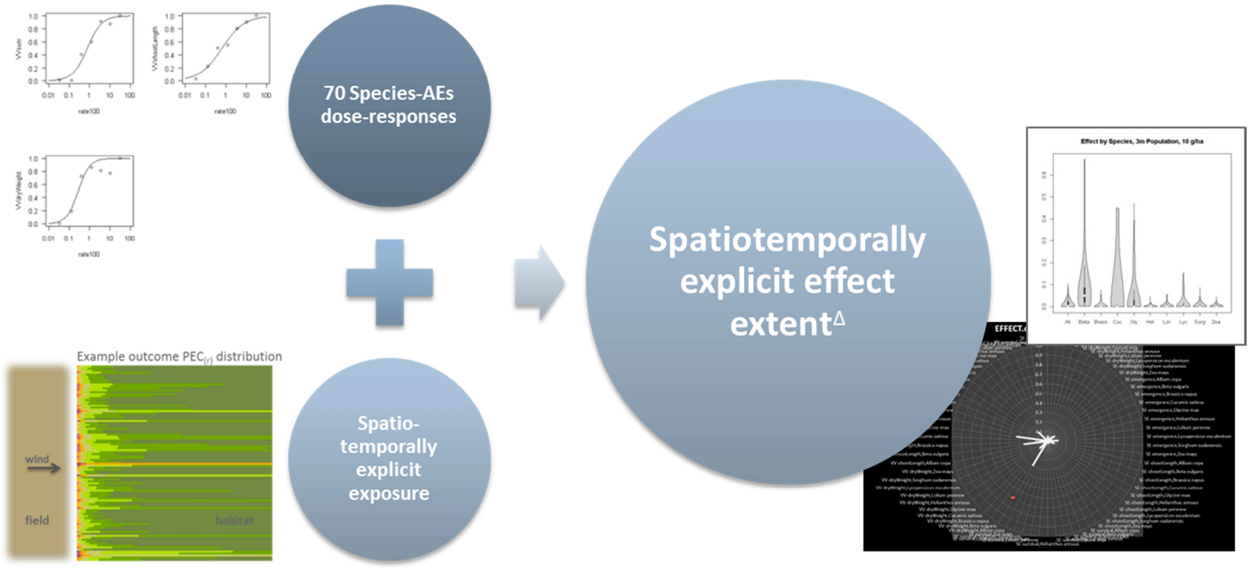


Figure 57: Overview on Step-1 risk characterisation.

The evaluation of outcome of the spatiotemporally explicit exposure and effect assessment ('Step-1' analysis, *Xplicit-NTTP-Model*, Section 6.2.4.5) included an aggregation step over time, by which the maximum effects over the simulation period were obtained. The remaining distributions of individual-level effects comprised 3-dimensions: *species*, *AE* and *space*. These were evaluated for the edge-of-the-field- and regional-scale.

The risk characterisation for the 3-dimensions *species*, *AE* and *space* was done in three steps:

i. *Effects* not differentiated by any dimension: *Effect()*|$_{(space,\ species,\ AE)}$.

   In first approximation, this can be interpreted as 'response of all individuals of a community', showing effects irrespective of where they occur, for which species or for which *AE*.

ii. *Effects* differentiated by *species* or by *AE*:

   Effect(species)|$_{(space,\ AE)}$, *Effect(AE)*|$_{(space,\ species)}$

iii. *Effects* differentiated by *species* and by *AE*: *Effect(species, AE)*|$_{(space)}$

   This evaluation shows the most detailed picture of the distribution of individual *species* and *AE* responses over the spatial extent of the community.

6.2.4.4 GeoData

Two exemplary landscapes of different scales were employed (Figure 58):

i. Scale-1, edge-of-the-field-scale:
   - Schematic 1 ha square field with local edge-of-the-field NTTP community of different sizes: 100 m x (3 m, 5 m, 10 m, 50 m, 100 m).
   - NTTP community downwind (no variability of wind direction).
   - Spray-drift deposition variability (Section 6.2.4.5).

ii. Scale-2, regional-scale:
   - Real-world agricultural region dominated by arable (Münsterland, Germany) with (small) herbaceous plant communities in-between. Land use / cover characterised from high-resolution aerial imagery (≈0.5 m, GeoContent 2012) using object-based image analysis software (eCognition, Trimble 2012).
   - Focus on herbaceous plant communities occurring in field vicinity (Figure 59).
   - Variability of wind direction (Section 6.2.4.5).
   - Variability of spray-drift deposition (Section 6.2.4.5).

Further generated artificial edge-of-the-field scenarios, as well as real-world landscapes from different regions in Europe are under investigation.

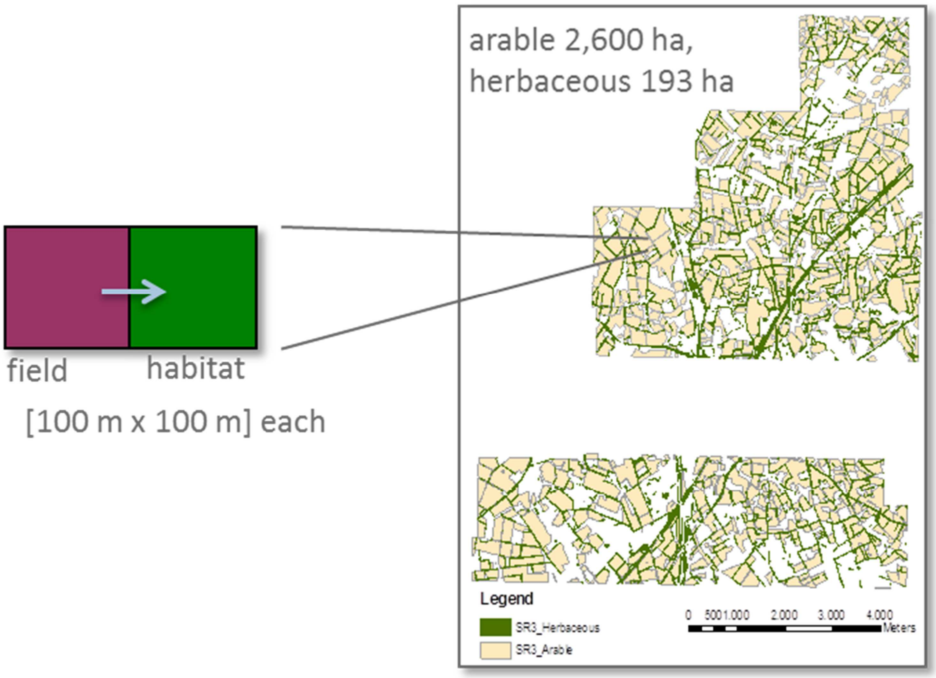


Figure 58: Study landscapes: Edge-of-the-field (left, arrow indicates wind direction) and regional-scale (right, Münsterland, Germany).

Figure 59: Illustration of field margin vegetation (images) and its occurrence in the regional-scale test geodata (map, green stripes).

6.2.4.5 Xplicit-NTTP-Model

Spatiotemporally explicit exposure and effect assessment as well as appropriate aggregation of results was done using an *Xplicit-NTTP-Model* (definitions summarised in Table 20). The *Xplicit-NTTP-Model* was derived from the *Xplicit-Framework* (Section 5.3).

Table 20: Definitions of the *Xplicit-NTTP-Model.*

Entity	**Definition**
Key study entities	PPP application areas (arable fields) and NTTP areas.
Landscape geodata	Land use/cover: (i) Schematic edge-of-the-field-scale scenarios (*e.g.*, 1 ha square field with 1 ha square NTTP area downwind); (ii) real-world land use/cover of arable cultivation region in Germany (high-resolution).
Receptors	• Abiotic: NTTP area segments (receptors) from discretisation of land use/cover geodata (1 m x 1 m for edge-of-the-field-scale, 2 m x 2 m for real-world scenarios). • Biotic receptors represent 10 ecotoxicological test species and 7 *AE*s.
PPP use	Single application of a herbicide to arable (post-emergence) at 100 g a.s./ha

Entity	Definition
	using 90% spray-drift reducing application technology. Application timing was not a relevant parameter as predefined conditions of Tier-1 RA level were kept (*e.g.*, vegetation development vs. PPP use).
Exposure	• Distance dependent spray-drift deposition taking variability of local depositions into account (Golla *et al.* 2011). • For edge-of-the-field-scale scenarios, NTTP areas located downwind, *i.e.*, no variability regarding wind direction. • For real-world landscapes, local spray-drift deposition depended on crop-to-NTTP segment (receptor) distance and on wind direction: deposition occurred downwind; *Exposure-Paths* represent potential wind directions (Section 5.3.5.3, Figure 31); 8 wind directions of equal probability considered (compass directions N, NE, E, SE, S, W, SW); for each application a random wind direction per field was selected. • Spray-drift deposition reached NTTPs as defined in the Tier-1 scenario (*e.g.*, no interception due to vegetation structure, no filtering by intervening vegetation). • Superposition of spray-drift deposition into a single NTTP segment (receptor) from different neighbouring fields possible.
EFate	• In case of multiple spray-drift depositions onto a single NTTP segment (receptor), exposure was added to already existing residues (no dissipation of the substance on NTTPs (DT50 = 9999 days).
Effect	• Effect data were taken from a 'Vegetative Vigour (VV)' and a 'Seedling Emergence (SE)' study, which provided data for 10 species and 7 *AEs* each (emergence (SE), survival (SE, VV), dry weight (SE, VV), shoot length (SE, VV)). Dose-response curves were calculated for 70 *species-AEs* from the data (log-logistic) using the R-Statistics 'DRC-package' (CRAN 2012).
Monte Carlo	• Monte Carlo (MC) approach with N=30 MC runs. • In each MC run for each receptor exposure and effect level were calculated by daily time-steps.
Risk Characterisation	• Expectancy values for percentiles of PEC and effect level, by different groups (all *species-AE*s, by species and by *AE*s, by individual *species-AE*s). • Risk characterisation for edge-of-the-field and regional-scale scenarios, taking different NTTP community sizes as base assessment units into account (width of NTTP area, *e.g.*, 3 m, 5 m, 10 m, 3 m – 10 m, etc.). • For each MC run (out of *N*) the distributions of exposure (PEC) and effect over the receptors were evaluated by calculating location parameters (percentiles, *e.g.*, 90th percentile PEC, P90 effect). From the *N e.g.*, P90 effect expectancy values were calculated.

6.2.4.6 Ecological Modelling

Mechanistic ecological modelling provides means to move risk characterisation of NTTPs from the *Individual*-level to the plant population or community level, which are the actual biological entities of protection goals (EFSA 2010a).

A preliminary literature review was conducted aiming at the identification of model approaches that correspond to the following criteria:

- The model should operate spatially and temporally explicit.
- The model should consider potential competition between plants (*e.g.*, surface, soil).
- Individual Based model approach (IBM) preferred.
- Preferred plant community types are herbaceous communities, which typically occur in cultivated landscapes in central Europe.
- Representation of plant community as (functional) traits would be favourable.
- The model should be capable of taking effects of environmental conditions (*e.g.*, nutrition, weather) to plant development into account.
- Model scales should fit to target scales in SPGs, hence, in refined risk characterisation (*e.g.*, spatial range ≈10^0-10^4 m^2, temporal ≈days-years).
- Model validation should be considered.

The literature search revealed a single promising approach published by May, *et al.* (2009). A presentation and discussion of the model (Prof. Jeltsch, University Potsdam) at Bayer CropScience (2012, Figure 60) underlined its potential applicability in context of the objectives of this study. The model will therefore be used in Step-2 (Section 6.2.4.3). This knowledge on the overall project design was incorporated in the definition of the present case study (Step-1).

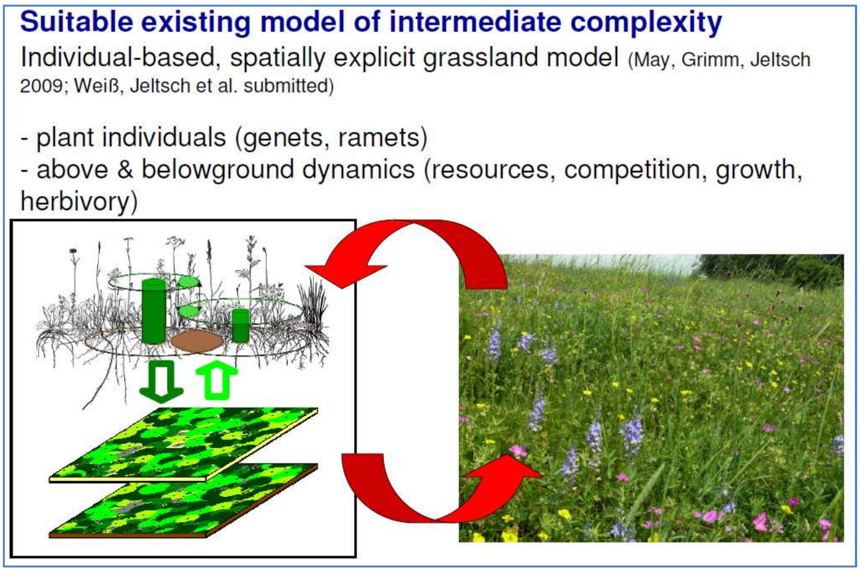


Figure 60: Plant community model proposed by F Jeltsch (presentation at Bayer CropScience, August 2012, with the kind permission of the author F Jeltsch, University Potsdam).

6.2.5 Results and Discussion

Results for the exposure and the individual-level effects are summarised below. Presented endpoints, *e.g.*, 90th percentile effect (P90) are expectancy values '<P90 Effect>' derived from Monte Carlo runs (Section 6.2.4.5).

6.2.5.1 Co-occurrence of Arable Fields and Non-Target-Terrestrial Plants

Spatial relationships of the co-occurrence of arable fields and NTTPs show initial insights on potential risk and provide a basis for consistency check and interpretation of spatiotemporally explicit risk characterisation using Xplicit.

For edge-of-the-field-scale scenario with schematic landscapes (Figure 58) spatial relationships are apparent. Simple spatial analysis (GIS) on the co-occurrence of NTTPs and arable fields for the region 'Münsterland' (Figure 58) shows that about 35% of herbaceous areas occur in ≤3 m distance from arable fields (47% in ≤5 m and 62% in ≤10 m distance). Thus, large fractions of the NTTP areas occur in distances to fields for which significant spray-drift exposure can occur.

The data underline the intense cultivation characteristics of the test region. Besides their high vicinity to arable fields, herbaceous NTTP areas are typically of small width (≈5-8 m, rarely >10 m). For the objectives of this case study, larger NTTP areas like meadows were intentionally not considered. The herbaceous NTTP areas are often surrounded by fields.

Therefore, the test region can be regarded a conservative landscape scenario with respect to potential exposure of NTTP communities due to spray-drift, given by the close field-to-NTTP occurrence, the high fraction of NTTP areas in close vicinity, their low spatial extent (no large NTTP area like meadows), as well as the high spatial interspersion of NTTP areas and fields.

6.2.5.2 Spatiotemporally Explicit Individual Level Effects

Individual-level effect data were taken from a 'Vegetative Vigour (VV)' and a 'Seedling Emergence (SE)' study, in which seven *AEs* were tested (emergence (SE), survival (SE, VV), dry weight (SE, VV), shoot length (SE, VV)) (Section 6.2.4.1).

The evaluation of outcome of the spatiotemporally explicit exposure and effect assessment ('Step-1' analysis, Section 6.2.4.3, *Xplicit-NTTP-Model*, Section 6.2.4.5) included an aggregation step over time, by which the maximum effects over the simulation period were obtained. The remaining distributions of individual-level effects comprised 3-dimensions: *species*, *AE* and *space*. These were evaluated for the edge-of-the-field- and regional-scale.

Edge-of-the-field-Scale

Different NTTP community widths were investigated (*e.g.*, 3 m, 5 m, 10 m, 3-10 m, Section 6.2.4.5), starting at 1 m distance from the field boundary (Rautmann *et al.* 2001). The 3 m width community is referred to as '*Close-Field-Margin*', that of 3-10 m as '*Distant-Field-Margin*'.

Following the objective of presenting this case study in context of this thesis, the presentation is focused on a few representative results and their discussion. All results shown herein are consistent with the entirety of findings that have been obtained so far.

Figure 61 and Figure 62 show cumulative distributions of effects not differentiated by any dimension (*Effect()*$|_{\text{(space, species, AE)}}$, evaluation level (i), above).

- For the most conservative *Close-Field-Margin* community (Figure 61), 90% of individual effect responses are <0.05 (5%) effect level. More than 70% of individual effects across the plant community are <0.01 (1%) effect level. Very few cases (<1%) show effects >0.4 (40%) (see also below, evaluation step (iii)).
- For the *Distant-Field-Margin* community (Figure 62), 90% of individual effect responses are <0.02 (2%) effect level. More than 80% of individual effects across the plant community are <0.01 (1%) effect level. Very few cases (<1%) show effects >0.4 (40%).
- The observed effects are a result of the distribution of exposure over the plant community extent, the 10 species, and the 7 *AEs*, as well as the shape of the individual dose-response relationships (70 *species-AE*s in total).
- The resulting distribution of such 'anonymous' effects over a small plant community occurring at the edge-of-the-field preliminary indicates that a limited fraction of the plant community showed high individual effects. However, at this risk characterisation level, it remains unclear whether the nature of these effects can lead to significant effects at plant population or community level.

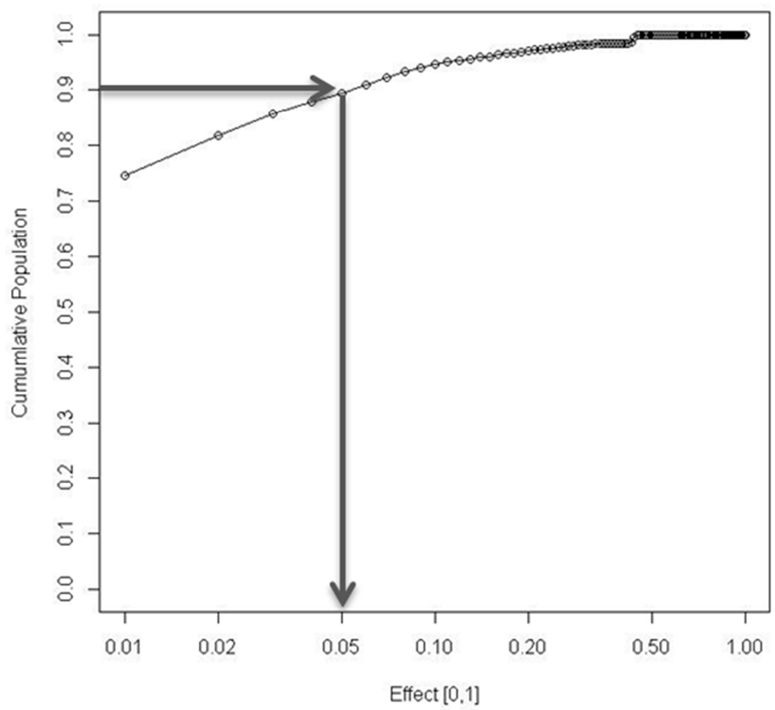


Figure 61: Distribution of effects of the *Close-Field-Margin* community (3 m width, starting at 1 m from field edge) obtained for the edge-of-the-field-scale scenario (cumulative). *Effects* not differentiated by any dimension: *Effect()*$|_{\text{(space, species, AE)}}$.

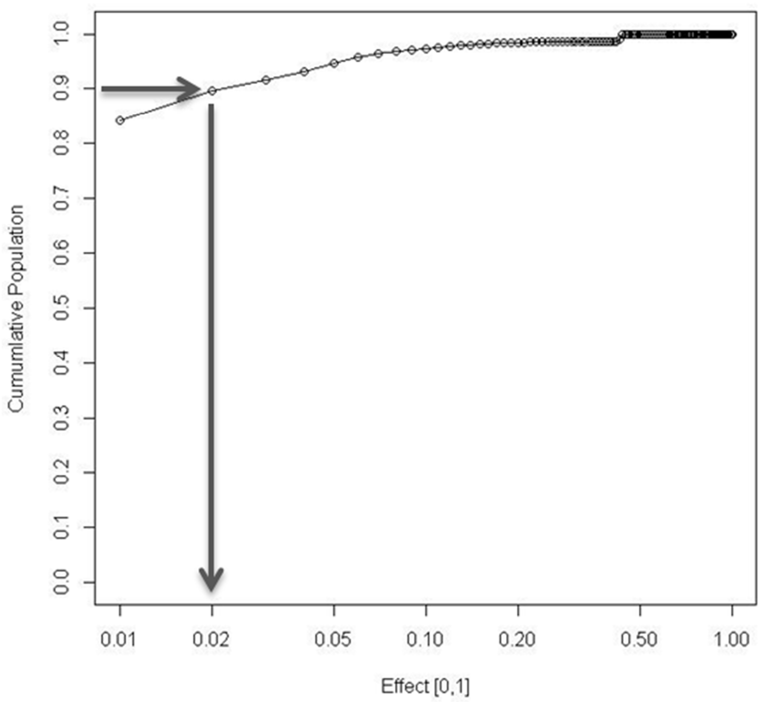


Figure 62: Distribution of effects of the *Distant-Field-Margin* community (3-10 m width, starting at 1 m from field edge) obtained for the edge-of-the-field-scale scenario (cumulative). *Effects* not differentiated by any dimension: *Effect()*$|_{\text{(space, species, AE)}}$.

Analysis of effects by *species* (without differentiation of *AE*, *Effect(species)*$|_{\text{(space, AE)}}$), and by *AE* (without differentiation of *species*, *Effect(AE)*$|_{\text{(space, }species\text{)}}$) showed that major individual effect responses originate from 2 of 10 species and from a few sublethal effect types (see also below, evaluation step (iii)).

In Figure 63 and Figure 64, *Effect(species, AE)*$|_{\text{(space)}}$ are shown, *i.e.*, effects are differentiated by *species* and by *AE*, hence, only distribute over the spatial plant community extent (*space*). Presentation of results is focused on the most conservative *Close-Field-Margin* community. In Figure 63, the 90th percentile of the distribution of effects by *species* and *AE* over the plant community is shown (<P90 effect>), Figure 64 shows the 50th percentile (<P50 effect>).

- The radial plot provides a good visual impression of the variability the effect profile over *species* and *AE*. The plots indicate that from the 70 *species-AEs* of the plant community only a small fraction showed pronounced individual-level effects, among which sublethal are dominating.
- 90% of the *Close-Field-Margin* community showed less or equal effect levels shown in Figure 63. At 90th percentile of the community extent, 2 *species-AE* showed ≈0.3 effect level (30%), both of which are sublethal. Two survival effects of 0.1<effect<0.2 were observed. In total, 6 of the 70 *species-AEs* showed effects of 0.1<effect<0.4.
- 50% of the *Close-Field-Margin* community showed less or equal effect levels shown in Figure 64. At 50th percentile of the community extent, a single *species-AE* showed effects of 0.2<effect<0.3 (20%-30%, sublethal). Survival effects of effect>0.1 were not

observed. In total, 3 of the 70 *species-AE* showed effects of 0.1<effect<0.3, none of which were survival effects.

- This effect profile depends on the mode of action of a herbicide and the sensitivity of the selected species.

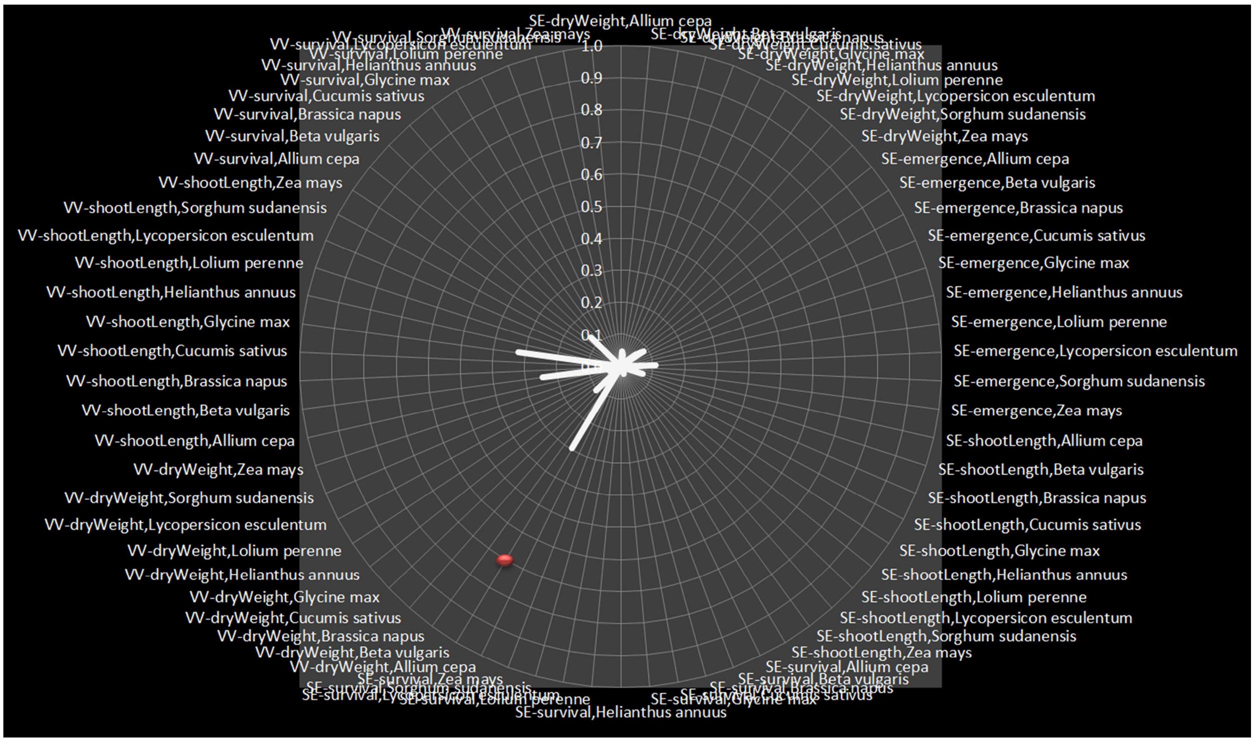


Figure 63: 90th percentile of effect distribution of the *Close-Field-Margin* community by *species* and by *AE* (*Effect(species, AE)*$|_{(space)}$) (Ordinate: effect level, red dot = Tier-1 effect value).

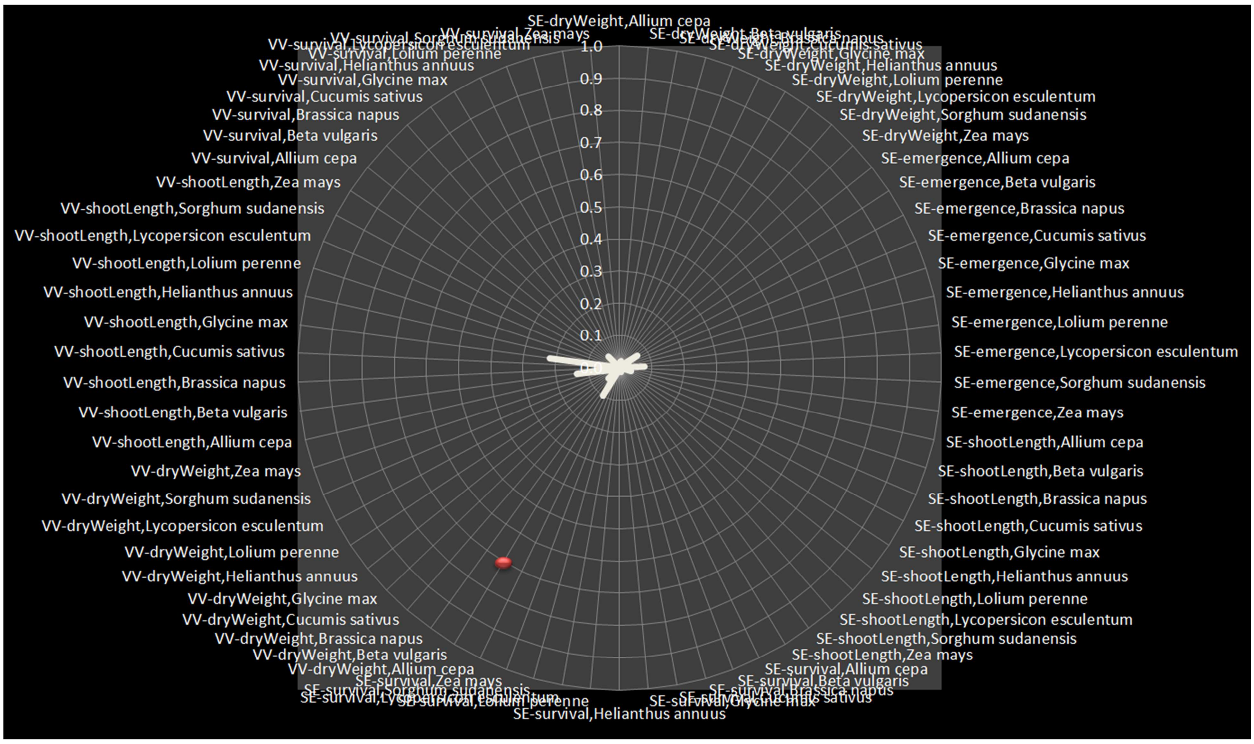


Figure 64: Median of the effect distribution of the *Close-Field-Margin* community by *species* and by *AE* (*Effect(species, AE)*$|_{(space)}$) (Ordinate: effect level, red dot = Tier-1 effect value).

<u>Regional-Scale</u>

As introduced in Section 6.2.4, a dense arable test-landscape (Münsterland) was investigated. As an additional conservative definition, only herbaceous NTTP communities were assessed, which is conservative as this type frequently occurs in close vicinity to fields and is typically of small spatial extent (compared to other NTTP community types like meadows or grassland).

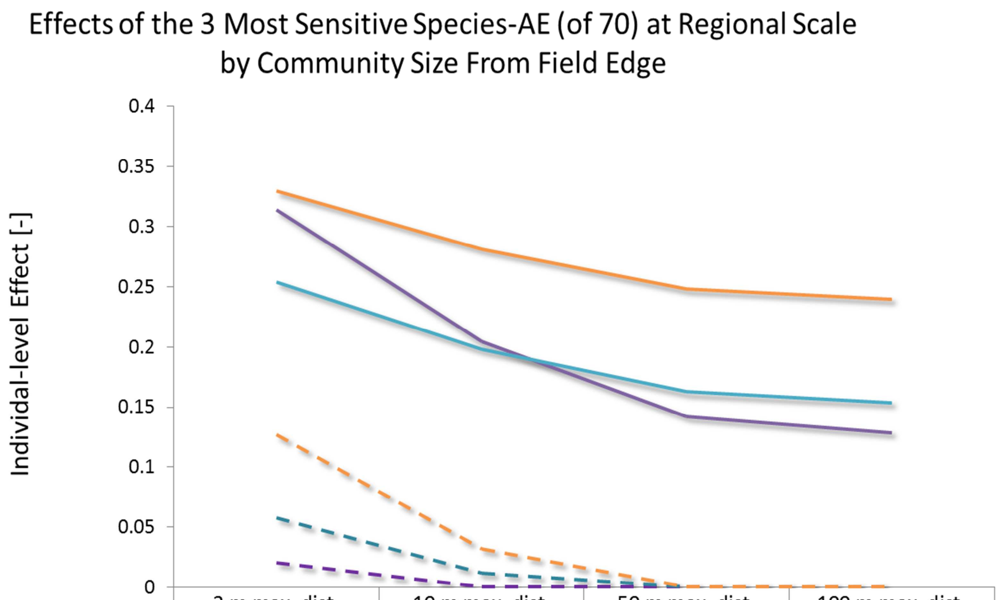
Results are presented for the three most sensitive *species-AE* responses (Figure 65). Other *species-AE* responses were significantly lower, with a general pattern similar to the one obtained in the edge-of-the-field-scale analysis above (Figure 63, Figure 64).

Four different NTTP communities sizes were assessed, starting at 1 m from field edge, and extending up to maximum distances of 3 m, 10 m, 50 m and 100 m (Figure 65).

- Preliminary risk characterisation for small herbaceous NTTP communities occurring in immediate field vicinity in an intense arable landscape (represented by the 100 m maximum distances evaluation) demonstrates, that only a small fraction of the community show pronounced effects (individual level, sublethal). This essential result encouraged the question of whether sublethal effects on individual-level, limited in effect extent, limited to a fraction of species, Assessment Endpoints, and spatial extent can cause unacceptable effects at community level under real-world conditions.
- The 90th percentiles of all community sizes range close to those obtained at edge-of-the-field-scale. This indicates that at regional-scale parts of small plant community are of same conditions as at edge-of-the-field-scale. This is apparent as always parts of such

plant communities occur immediate to the field boundary and as herbaceous areas are of limited spatial extent. The influence of variability of conditions at regional-scale (*e.g.*, due to wind directions) is shown by the 50th percentile effects, which are significantly lower than at edge-of-the-field scale. Thus, the regional-scale demonstrates that even for small herbaceous plant communities occurring in immediate vicinity to fields in dense cultivations, natural variability of exposure conditions and landscape structure affects risk characterisation.

- The decrease of the 50th percentile with plant community size demonstrates the importance of habitat size, and hence, of landscape management (*e.g.*, structure) for the viability of (semi-) natural plant communities.



	3 m max. dist.	10 m max. dist.	50 m max. dist.	100 m max. dist.
Beta vulgaris - VV-dryWeight - P50	0.02	0.00	0.00	0.00
Beta vulgaris - VV-shootLength - P50	0.06	0.01	0.00	0.00
Glycine max - VV-shootLength - P50	0.13	0.03	0.00	0.00
Beta vulgaris - VV-dryWeight - P90	0.31	0.20	0.14	0.13
Beta vulgaris - VV-shootLength - P90	0.25	0.20	0.16	0.15
Glycine max - VV-shootLength - P90	0.33	0.28	0.25	0.24

Figure 65: 90th percentiles (<P90 effect>, solid lines) and median (<P50 effect>, dashed lines) effects of distributions of individual-level effect responses over NTTP communities of different size at regional-scale (*e.g.*, '10 m max. dist.' = community that starts at field edge (1 m), and extends up to a maximum distance of 10 m). Three most sensitive *species-AEs* shown.

6.2.6 Conclusions & Outlook

- Starting from the definitions and data at Tier-1 RA level, which was not passed by the test herbicide, the propagation of exposure variability to individual-level dose-responses of 10 species and 7 attributes provided a first level of quantitative risk characterisation. Quantification of effect extent was done for the three risk dimensions *species*, *Assessment Endpoint* (*AE*) and *space*, at edge-of-the-field- and regional-scale. As the case study design was developed on the basis of the Tier-1 scenario and carries characteristics of the Tier-1 level, results are considered immediately applicable to refine corresponding regulatory RAs.
- At the edge-of-the-field-scale, a small NTTP community of 3 m width occurring downwind from the field was assessed. Only a small fraction of the 70 endpoints (10 *species*, 7 *AEs*) of the plant community showed pronounced effects, among which sublethal were dominating: *e.g.*, at the 90th percentile of the spatial community extent, 2 *species-AEs* showed ≈0.3 effect level (30%), both of which were sublethal. Two survival effects of 0.1<effect<0.2 were observed. In total, 6 of the 70 *species-AEs* showed effects of 0.1<effect<0.4. At 50th percentile, a single *species-AE* showed effects of 0.2<effect<0.3 (sublethal). A single survival effect of 0.1<effect<0.2 was observed. In total, 3 of the 70 *species-AE* showed effects of 0.1<effect<0.3 (sublethal).
- At regional scale, a test landscape of dense arable cultivation was investigated. Only herbaceous NTTP communities were assessed, which is conservative as this type frequently occurs in close vicinity to fields and is typically of small spatial extent, compared to, *e.g.*, meadows. Four different NTTP community sizes were assessed, starting at 1 m from field edge, and extending up to maximum distances of 3 m, 10 m, 50 m and 100 m. Parts of plant communities were found of same risk as at edge-of-the-field-scale. This is apparent, as always parts of such plant communities occur immediate to the field boundary. The influence of variability of conditions at regional-scale (*e.g.*, due to wind directions, landscape structure) is shown by the 50th percentile effects, which are significantly lower than at edge-of-the-field scale. Thus, the regional-scale analysis demonstrates that even for small herbaceous plant communities occurring in immediate vicinity to fields in dense cultivations, natural variability of exposure conditions and landscape structure affects risk characterisation.
- At regional scale, the decrease of the 50th percentiles with plant community size demonstrates the importance of habitat size, and hence, of landscape management (*e.g.*, structure) for the viability of (semi-) natural plant communities.
- Preliminary risk characterisation for small herbaceous NTTP communities occurring in immediate field vicinity in an intense arable landscape demonstrates that only a small fraction of the community shows pronounced effects (individual level, sublethal). This essential result encouraged the question of whether sublethal effects on individual-level, limited in effect extent, limited to a fraction of species, Assessment Endpoints, and spatial extent can cause unacceptable effects at community level under real-world conditions.

- Steps towards risk characterisation at plant population and community level were outlined and an *Individual-Based-Model* was identified (May *et al.* 2009) to propagate the obtained individual-level effects over *species*, *Assessment Endpoint* (*AE*) and *space* to the community level, as the biological entity at which SPGs are targeting (EFSA 2010a, 2010b). Beyond its immediate value, this assessment level will also allow to further specify risk characterisation for biodiversity protection goals.
- Methods and data as employed in the case study can also support the development of future RA scenarios (at different tiers) with quantified protection levels. The complexity of interacting processes, *e.g.*, variability of wind directions and local habitat-to-field distances, landscape structure, species- and Assessment Endpoint-dependent number and shape of the dose-response functions, emphasises the necessity of spatiotemporally explicit and probabilistic approaches (Xplicit), taking scale dependencies into account.
- Beyond the methods and data used in this pilot study, quantification of risk of NTTPs can be further refined by processes describing spray-drift depositions in 3-dimensional vegetation structures more realistically. Also, further exposure routes can be taken into account (*e.g.*, run-off). Generated artificial landscapes of defined characteristics can be used to generically investigated relationships between landscape structure and potential risk.
- Species composition and abundance in plant communities are generally influenced by environmental conditions and competition (Ellenberg *et al.* 1992). Especially small herbaceous plant communities, occurring in agricultural landscapes are affected by a number of conditions besides herbicidal effects, *e.g.*, habitat sizes, connectivity/isolation, fertiliser, maintenance, mechanical effects, landscape dynamics, etc. Therefore, the *SynContext* viewpoint (Section 4.2), which sets the ecological system (here, the plant community) in the centre of the assessment, can support the development of efficient management strategies to achieve protection goals (Section 6.2.3.1, 4.3.2).

6.3 Risk Characterisation for Aquatic Plants for the Use of a Herbicide on Rails in UK

This case study presents an example use of the Xplicit approach with a large geodataset covering relevant entities for an entire country. On this basis, insights on risk of aquatic plants due to spray-drift entries from the use of a herbicide on rails could be developed which was not possible with the standard RA approach.

6.3.1 Lessons Learned

- Starting at the standard Tier-1 RA, which does not quantify risk extent, the landscape-scale risk characterisation establishes a new basis for regulatory RA and RM decisions.
- The Xplicit concepts and approach, including adequate geodata, spatiotemporally explicit and probabilistic exposure and effect calculation, as well as evaluation of simulation outcome at ecologically meaningful scales, can provide a clear and quantitative basis for RA and RM that fits to SPGs (EFSA 2010a, Section 4.3.2.1).
- Refined risk characterisation can directly be used for PPP-specific RM by local adaptation of the PPP use rate according to WB vulnerability using a Global Positioning System (GPS). Local vulnerability can also be subject to generic RM measures (*e.g.*, adaption of WB maintenance, improvement of riparian vegetation).
- The Xplicit approach provides a means for scenario development in context of SPGs (Reference Scenarios, EFSA 2010a). The case study already includes first steps towards *SynContext* (Section 4.1) by assuming 100% PPP use on all rails and 100% market share.
- The study demonstrates that refined risk ecological risk characterisation can be achieved with manageable effort (data, processing, evaluation, reporting). In a quality check procedure, small-scale geodata were improved using data enhancement concepts (Section 6.4.7).
- Risk characterisation was done using standard ecotoxicological data which refers to the individual-level. Ecological modelling means (Section 5.3.5.7) are proposed to be used as effect models in *Xplicit-Models* in order to characterise risk at population and community level.
- Targeting at risk characterisation in SPG context, the Xplicit approach can support the ('*a posteriori*') definition of SPGs in sense of providing a preliminary empirical basis of risk extent under more realistic conditions, *e.g.,* in terms of spatial and temporal risk extent.
- The study showed the adaptability of the *Xplicit-Framework* approach to a specific problem formulation, resulting in an *Xplicit-Rail-Model*.

6.3.2 Abstract

Railway maintenance includes the use of herbicides by spray application to control weeds. Such spray application is accompanied with a fraction of the sprayed volume drifting from the actual application zone (railway) and potentially deposit into neighbouring water bodies (WBs). The standard Tier-1 RA level (HardSpec model, Hollis 2010) assumes the WB located close and downwind to the rails with no further protection against spray-drift deposition (*e.g.*, no riparian vegetation). For a given herbicide ('Herbicide-1') this assessment level resulted in a TER<1, which indicated unacceptable risk, yet, without quantifying risk extent or offering RM options.

The present study aimed at refined risk characterisation for aquatic plants due to spray-drift of Herbicide-1 when used on railways in the UK. Risk driving environmental factors *distance* and *wind direction* were refined using geodata on the occurrence of railways and WBs across UK, variability on possible wind directions, and the Xplicit approach.

In absence of SPGs for aquatic plants a proposal for risk characterisation targets was developed. Ecotoxicological effect characterisation was kept as determined at Tier-1 level (NOAEC, TER approach, with a TER<1 indicating unacceptable effect). The aquatic plant (meta-) population was considered as target biological entity. On this basis, the spatial extent of TER<1 occasions represented (meta-) population effects. Temporal risk extent was not explicitly refined, but was kept at Tier-1 level, as the maximum exposure and effects over the simulation period were assessed, and as a TER<1 occasion was considered as a permanently lasting effect.

A '*Xplicit-Rail-Model*' was implemented from the *Xplicit-Framework* (Section 5.3). The farmer module represented Herbicide-1 applications on railways. The exposure module used a distance-dependent spray-drift deposition function derived from the empirical data of the HardSpec model (Hollis 2010) and random wind directions (even PMF of eight compass directions). The eFate module reflected the WB definition of the HardSpec model. A *Landscape-Metric* service provided data on local direction-dependent rail-to-WB distances.

In a spatial analysis step the occurrence of WBs in the vicinity of rails was assessed as an initial examination on potential risk and for consistency check for the detailed risk characterisation. An approximate distance at which spray-drift depositions can potentially lead to unacceptable effects to aquatic plants (TER<1) is 20 m. From all WBs occurring within 1 km from rails, 2% of their length occur within such a distance. 94% of individual WBs in up to 1 km distance have <10% of their length closer than 20 m to rails. Thus, potential exposure of WBs due to spray-drift from rails is limited to small fractions of the entire WB set and individual WB length.

Spatially explicit PECsw and TERs were calculated for each 5 m WB segment ('receptors') using the *Xplicit-Rail-Model*. Outcome was assessed at two scales: (i) 'WB_{pooled} – scale', by pooling all WBs occurring in the vicinity of rails in a single set, and (ii) '$WB_{individual}$ – scale', for each individual WB occurring in the vicinity of rails. The outcome was assessed for four WB groups of different spatial extent, including WBs within 1 km, 500 m, 200 m, 100 m from railways.

At WB_{pooled} – scale, *i.e.*, assessing the entirety of WBs without distinguishing individual WBs, the vast majority of WB segments are unlikely to receive spray-drift depositions that result in a TER<1: *e.g.*, a TER<1 was obtained for <<1% of WB segments in 1 km WB group (<5%, 100 m WB group). At $WB_{individual}$ – scale, it was found that TER<1 occasions occurring at large extent of an individual WBs are rare, *i.e.*, aggregation of effects in individual WBs is infrequent. This is

first of all as typically WBs only occur with small fractions of their length close to railways (*e.g.*, intersecting rails) and as natural WBs (*e.g.*, streams, ponds) apparently mainly occur at considerable distances. In an additional analysis, and for demonstration purposes, potential effects of spray-drift filtering by riparian vegetation were taken into account, which further reduced exposure and risk by 60%.

Results of the spatiotemporally explicit RA significantly improved risk characterisation, and provide a basis directly applicable for RM. This was achieved by characterising risk at the scale individual WBs, expressed in terms of the probability that a quality criteria is violated, *e.g.,* P(TER<1 for >10% of WB length). In case RA reveals unacceptable risk, the protection of potentially vulnerable WB sections can be improved as their locations and vulnerability level are known. RM options are, *e.g.*, locally adapting the herbicidal use rate (up to switching-off) or by a generic RM campaign (*e.g.*, adaptation of WB maintenance). As the results suggest, the absolute number of such vulnerable WB sections appears comparably small, hence, RM efforts appear manageable.

Further research is primary suggested on the definition of adequate SPGs for aquatic plants, and so, on defining a basis for adequate risk characterisation and risk communication. Efforts towards effect assessment on plant (meta-) population level are proposed, *e.g.*, by linking spatiotemporally explicit exposure to ecological modelling (Section 5.3.5.7). Also, means to refine the characterisation of substance environmental fate (eFate) in aquatic networks should be evaluated.

6.3.3 Introduction & Objectives

Railway maintenance includes the use of herbicides to control weeds. Herbicide application on rails in the UK is typically done by spray application with the 'Radiarc' nozzle system (Hollis 2010, Hollis *et al.* 2004), installed on a rail wagon. A fraction of the sprayed volume can drift from the actual application zone (railway) and can deposits into neighbouring WBs.

In the worst-case, aquatic habitats populated with the plant species, most sensitive to the herbicide, are located close and downwind to the rails and are unprotected against spray-drift deposition. This scenario is approximately reflected for aquatic organisms in the HardSpec model (Hollis 2010) and builds the basis of the standard Tier-1 RA. In case this protective RA level indicates potential risk, the RA needs to be refined using more realistic data and model approaches. Lower-tier (*e.g.*, Tier-1) assessment levels are basically protective, and hence, are not designed to allow for detailed and quantitative risk characterisation.

The decision-making process in ecological RA for PPPs revolves around the question "*is risk acceptable?"*. In order to assess this, (i) it need to be defined how risk is to be characterised (in terms is ecotoxicological effects and their probability to occur), and (ii), what risk level would be acceptable. Both, phrasing of acceptability criteria and risk characterisation need to match in their design (*e.g.*, structure, semantics, endpoints, dimension, etc.).

A step towards Specific Protection Goals (SPGs) was presented by EFSA (EFSA 2010a, Section 4.3.2.1). In the present study, the (meta-) population was assumed to be the focus biological entity for non-target aquatic plants. Accordingly, risk characterisation referred to spatial dimensions which relate to plant (meta-) populations.

Landscape-scale approaches offer different aspects to improve RA with regard to closing the gap between protection goals and risk characterisation. This is achieved, *e.g.*, by assessing the spatiotemporal dimensions of risk, by using real-world data on environmental and PPP use conditions, and by taking different scales into account. Also, landscape-scale risk characterisation provides a means to evaluate alternative RM options. These aspects correspond to the goals of the *Xplicit-Framework* development (Section 5, Schad & Schulz 2011) which is used herein to derive a specific *Xplicit-Rail-Model*.

6.3.4 Data and Methods

Spray-drift deposition on aquatic habitats resulting from PPP use on rails is largely driven by two environmental factors (besides technical ones): distance between application area and aquatic habitats, as well as wind conditions. For a local WB segment, the direction-dependent distance to rails largely determines potential risk. Accordingly, risk of aquatic plant populations is likely to be of high spatiotemporal variability.

6.3.4.1 Summary on Processing Steps

Table 21 provides an overview on the major processing steps.

Table 21: Sequence of major processing steps.

Step	Short Description
Problem formulation	For the use of a herbicidal product ('Herbicide-1') on rails in UK, the standard lower-tier RA indicated unacceptable risk for non-target aquatic plants due to spray-drift depositions (TER<1). Standard Tier-1 scenario definition is protective and does not allow for risk quantification. Potential risk of aquatic plants due to spray-drift deposition from the use of Herbicide-1 on rails in UK has to be characterised using real-world data to refine key risk driving factors. A spatiotemporally explicit approach has to be used that allows to assess dimensions of risk with respect to protection goals.
Approach definition	Using adequate UK-wide geodata, the co-occurrence of rails and WBs was characterised spatially explicit and in appropriate detail. In a first step, a GIS analysis was conducted to quantify the co-occurrence of rails and WBs. In a second step, spatiotemporally explicit modelling was conducted to assess risk extent at appropriate scales. The Xplicit approach was used together with a distance-dependent spray-drift deposition model.
Data acquisition	Different data sources were evaluated. Data from OpenStreetMap® (OSM) and its verification built the basis of the analysis.
Data preparation	Presence and characteristics of rails and WBs given in OSM data were verified against high-resolution remote sensing data. Rails and WBs were well represented in the OSM data. As a conservative design, intervening vegetation acting as a filter for spray-drift was not considered in the main assessment.
GIS analysis	In a co-occurrence analysis the potential of rails to expose and the potential of WBs to get exposed was analysed using GIS.
Xplicit simulation	Risk extent and probability were calculated using the Xplicit approach for spatiotemporally explicit, probabilistic RA (Section 5.3, Schad & Schulz 2011).
RA	Results of the GIS and Xplicit analysis were compiled and summarised into a refined RA for aquatic plants for the use of Herbicide-1 on rails in UK. TERs were calculated from the exposure values as done in the standard Tier-1 assessment. Results were presented in straightforward percentiles, graphs and maps, and were discussed accordingly.

6.3.4.2 Active Substance

The ecotoxicological effect endpoint was derived from a mesocosm study defining the attribute and the magnitude of effects tolerated as ecologically 'no adverse' (NOAEC), same as determined in the RA process at Tier-1 level. A TER<1 indicated unacceptable effects.

Dissipation of the active substance was not taken into account. This allowed to conservatively assess superposition of depositions into the same WB (segment) resulting from applications on different neighbouring rails.

A single application of Herbicide-1 was assessed. All railways in UK were assumed to be applied with Herbicide-1. All applications were assumed to occur at the same day, using the 'Radiarc' nozzle system. All railways were conservatively considered double-track and both tracks were assumed to be treated with Herbicide-1.

6.3.4.3 Tier-1 Exposure and Risk Assessment

Tier-1 exposure assessment for the use of Herbicide-1 on rails resulted in a single peak caused by the spray drift event at day 0, which is based on the implemented drift curve for a spray train with Radiarc nozzles and default scenario distances and assumptions of the HardSpec 1.4.2 model (version 1.4.2, Hollis 2010, Hollis *et al.* 2004). The Tier-1 PECsw led in combination with an aquatic endpoint to a TER<1. Acceptable risk could not be demonstrated on Tier-1 exposure and RA level, and hence, a refined RA was necessary.

With respect to potential spray-drift losses during spraying and their deposition in the vicinity of rails, the HardSpec model makes the following scenario assumptions:

- 2 parallel railways (Figure 66).
- Both railways are treated by spray application with the 'Radiarc' nozzle system.
- Both treatments happen in the same time interval for which the peak deposition into an adjacent WB due to spray-drift is calculated.
- Minimum distance to WB of 5.14 m.
- Wind direction towards WB (*i.e.*, WB is located downwind).
- Considerable wind speed.
- No intervening or riparian vegetation that can act as a filter for spray-drift.

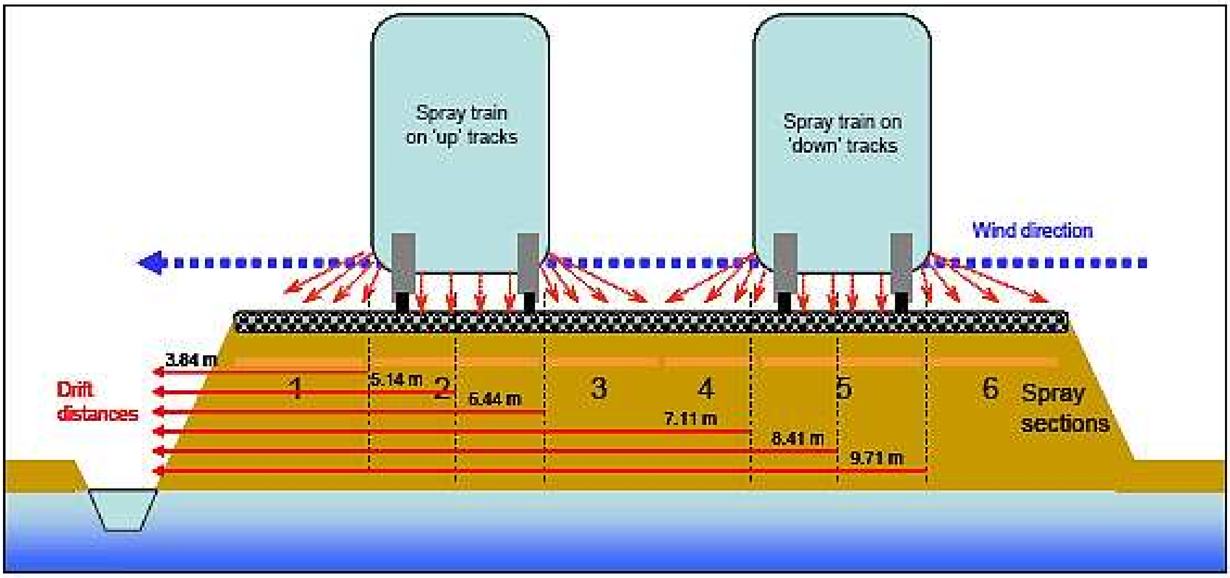


Figure 66: Spray-drift for the Railway surface water scenario (Hollis 2010, Hollis *et al.* 2004).

In the refined RA presented herein, basic scenario assumptions of the Tier-1 model for potential spray-drift entries into WBs were kept. This applies also for the minimum rail-WB distance of 5.14 m. The latter was confirmed by randomised measures taken on the basis of high-resolution remote sensing data (below).

Real-world conditions were introduced for

- the local rail-WB distance, used in a function representing percentage loss in dependence on rail - WB distance (below),
- and wind direction, due to the fact that wind can come from only one direction during spraying (*i.e.*, random wind directions were used).

All rails were conservatively considered double-line and both lines were assumed to be treated.

6.3.4.4 Deposition-Distance Regression

From the data given in the HardSpec model (Hollis *et al.* 2004, Hollis 2010) a distant dependent spray-drift deposition function was derived (Equation 12, y = fraction of application rate depositing [-], x = distance [m]) and was used in the exposure module of the *Xplicit-Rail-Model*. The function was referenced to point '2' of the Railway surface water scenario (Figure 66).

$$y = 0.9569x^{-1.3904} \qquad \text{Equation 12}$$

6.3.4.5 Data

Data to refine risk driving factors have a vital role in landscape-scale risk characterisation (*e.g.*, FOCUS Landscape & Mitigation recommendations, FOCUS 2007a, 2007b). According to the goals of the assessment, geodata on the occurrence of railways and WBs, in adequate quality, were of key importance. Ultimately, the geodatabases were intended to hold input information for spatiotemporally explicit probabilistic RA using Xplicit (Section 5.3).

Different data providers were approached including official institutes, commercial and open source (*e.g.*, UK Ordnance Survey (OS 2012), OpenStreetMap 2012 ('OSM'), ESRI data and maps (ESRI 2012), remote sensing data: Microsoft Bing (via esri GIS software, ESRI 2012, Google Earth Professional, Google 2012). Ultimately, OSM data were used.

To check for appropriate coverage of WBs and rails in OSM data, a quality check procedure was carried out, which comprised a manual verification against high-resolution remote sensing data (*e.g.*, Bing) using contingency tables. For a statistically sound sampling procedure, 1000 grids of 1 km² were randomly selected for each comparison. Different comparisons were conducted.

A first comparison using the complete OSM rail dataset showed that apparently a considerable number of rails were probably no longer in service and had been dismantled. Therefore, the dataset was adjusted by rails which were no longer in use (*e.g.*, rail types in OSM data: 'abandoned', 'disused', 'dismantled', etc.). In 1000 randomly sampled grids across UK no sample was found in which remote sensing data showed rails which were not contained in the pre-prepared OSM dataset. On the contrary, the comparison showed that in spite of having excluded rails attributed as no longer in use, the dataset still shows some over-representation of rails. This added to the conservatism of the study and did not form an obstacle to its use. Outside rail stations or urban areas, *i.e.*, across the country, double lined tracks were mostly represented by a single line in OSM. In the study, this was conservatively addressed by assuming that all rails were double-line in the exposure assessment. For the representation of rails, data verification had demonstrated that railways are well represented in the prepared OSM dataset.

In total, lengths of railways in the prepared OSM data set sums up to 22,284 km (Figure 67). This is higher than the value of 16,321 km which is reported by the International Union of Railways (UIC 2012) which is likely due to the fact that the International Union of Railways reports the length of the actual railway line (in a sense of a connection between two points), whereas the geographic OSM dataset represents physical rails, *i.e.*, including, *e.g.*, multiple tracks, platforms, freight yards, etc.

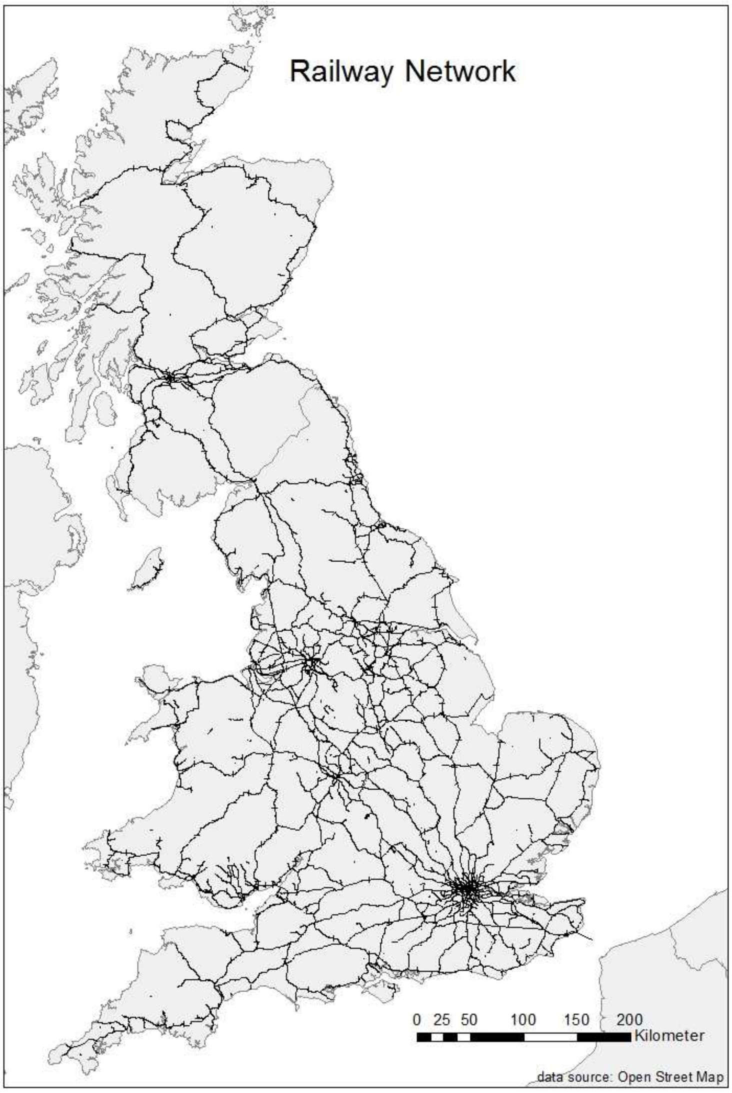


Figure 67: Railway network from OSM data.

The OSM WB dataset was compiled from the layers “waterways” (line) and “natural” (polygon). The latter included the types “water” and “riverbank” which were converted to bank lines, *i.e.*, as a conservative assumption for larger WBs only the bank line was assessed.

To assess OSM data quality concerning representation of WBs the same procedure than for rails was applied (above): 1000 1 km² grid cells containing rails were randomly selected (as for this project occurrence of WBs in rail vicinity was relevant) and conservatively examined for missing WBs: a grid was flagged as of 'missing WB' if *a single* section of a WB was missing in OSM. For 82 grid cells from 1000 (8%) missing WB segments were obtained. Therefore, for the goals of this study, it was concluded that WBs were adequately represented in the OSM.

Nevertheless, the 8% of cases where WB sections were missing triggered a more detailed analysis of the effect of missing WB sections to final RA. Therefore, entire railway tracks located in regions with high WB density were selected and WB features were manually digitised from high-resolution remote sensing data (or data represented in OSM were corrected) for railway tracks. The selection of the railway tracks based on the ratio of WB length in rail vicinity and rail length. 13 rails of highest index and considerable length were selected: Great Western Main Line, South Wales Main Line, Cambrian Line, Highland Main Line, Welsh Marches Line, Heart of Wales Line, Midland Main Line, Settle-Carlisle Railway, Newcastle and Carlisle Railway, Fen Line, Marshlink Line, Airedale Line, London to Penzance Main Line. For the 13 selected railways of a total length of about 1,524 km, 504 km of WBs were represented in the original OSM data and 550 km were found after manual adjustment. The effect of that 9% missing WB length to spatially explicit exposure and RA was investigated separately. The corrected WB dataset was incorporated into the final WB geodata used in the analysis which comprised WBs in up to 1 km distance from rails.

Linear WBs were represented by polylines in OSM. To ensure a conservative approach, from WB represented as polygon (areas), *e.g.*, ponds, lakes or larger rivers, only the outer riparian line was considered in the assessment, *i.e.*, larger rails-to-WB distances of the ponds' area or higher dilution due to large water volume was not taken into account in the calculations.

It is emphasised that the WB geodata contained a number of artificially (very) short individual WB sections. These artefacts are sections which are actually connected to further sections of an individual WB, yet, appear isolated due to *e.g.*, pipes, locks or intersections by roads.

In order to define ecologically meaningful basis for the RA of water plants, four different WB groups of different spatial extent were defined, which comprised WBs within 1 km, 500 m, 200 m, 100 m from railways.

6.3.4.6 Geospatial Analysis

The pre-processed geodata on rails and on WBs were analysed by means of GIS software (ArcGIS) in order to quantify the co-occurrence of rails and WBs. This simple spatial analysis was intended to provide a first indication on the potential risk by addressing the questions:

- *What is the potential of rails to represent an exposure source for spray-drift entries into WBs?* (rail perspective)
- *What is the potential of WBs to get exposed due to spray-drift entries from rails?* (WB perspective)

On the level of individual WBs, results of the geospatial analysis were evaluated also for the fraction of each individual WB (*e.g.*, stream, ditch, pond) that is located within 20 m from rails (the 20 m threshold was used as an indicator for potential effects as up to about this distance the spray-drift deposition curve derived from the Tier-1 exposure calculation resulted in TER<1). The aim of this analysis was to characterise the fractions of aquatic plant (meta-) populations that can be effected, and so, *e.g.*, to assess the recovery potential from within the same WB. It needs to be emphasised that this analysis is likely to be conservatively biased due to the fact that the geodata contains a number of artificially (very) short individual WBs. These are parts which are actually connected to further parts of an individual WBs, yet, appear isolated due to *e.g.*, pipes, locks or intersections by roads. Therefore, all analysis referring to individual WBs actually refer to WB *sections*, hence, can overestimate risk for individual WBs.

6.3.4.7 Explicit Risk Assessment

The second and major part the assessment concerned the spatially explicit calculation of local exposure and effects and a risk characterisation at scales meaningful to RA of aquatic plants.

A simple but adequate approach for risk characterisation was used.

The adverse effect to aquatic plants was represented by the Assessment Endpoint of the ecotoxicological experiments. For the sake of simplicity and to keep within the definitions of the standard Tier-1 assessment (NOAEC), the TER approach was employed as an indicator whether the adverse effect occurred: a TER < 1 represents an adverse effect.

The investigation of the extent of effects was guided by the EFSA opinion on Specific Protection Goals (EFSA 2010). For aquatic plants, the (meta-) population represents the ecologically most relevant biological entity at which protection goals can target. (Meta-) Populations of the sensitive plant species that built the basis of the ecotoxicological endpoint were assumed to occur in all WBs, *i.e.*, the (meta-) population as the biological entity of the assessment directly relates to the spatial extent of the WBs. Therefore, the risk dimension '*spatial extent*' built the focus of the analysis (at different scales, below).

In order to assess the spatial extent of risk, the spatial extent of effects, *i.e.*, TER<1 situations, and their probability to occur, had to be calculated. Providing a spatial extent of effects in absolute terms would be difficult to assess, as *e.g.*, an effect predicted at 20 m WB length would ecologically have a different relevance if it occurs per 100 m or per 1,000 m WB length, effect extent needed to be characterised in *context*. This context is provided by conducting the assessment at different spatial scales (below) which provide different ecological context to RA and RM, *e.g.*, a basis for considerations on recovery and recolonisation potential.

Two different '*ecological scales*' were defined representing ecological units:

(i) WB_{pooled} – scale: All WBs in the vicinity of rails pooled in a single unit.
(ii) $WB_{individual}$ – scale: RA by individual WB, *i.e.*, all individual WBs in the vicinity of rails.

These ecological units were assessed in different spatial scales, in which exposure and effect where set in context. Spatial scales were defined as four different WB groups which comprised WBs occurring within 1 km, 500 m, 200 m, 100 m from railways.

Temporal risk extent was not explicitly investigated. A local TER violation (TER<1) was taken as an unacceptable adverse effect event independent of how long it might last (kept as defined in Tier-1 assessment). Its potential temporary character, including substance dissipation and plant recovery, was not assessed, yet, can be subject to future refined risk characterisation.

6.3.4.8 *Xplicit-Rail-Model*

Risk characterisation as described above required spatiotemporally explicit exposure and effect calculation and appropriate evaluation of results. To this end, a '*Xplicit-Rail-Model*' model was derived from the *Xplicit-Framework* (Section 5.3, Table 22).

Table 22: Definitions of the *Xplicit-Rail-Model*.

Entity	**Definition**
Key study entities	PPP application areas (railways) and WBs.
Landscape geodata	Geodata representing railways and WBs across UK.
Receptors	• WB segments of 5 m length, representing habitats of Non-Target-Aquatic plants, discretised from WBs which were represented by lines (ponds are represented by the outer bank line). • WB definitions kept as in Tier-1 scenario (*e.g.*, depth = 0.3 m). • In the main analysis, WBs were assumed without riparian vegetation, *i.e.*, without protection due to spray-drift filter barrier.
PPP use	• Single application of Herbicide-1 on rails. 100% rails applied, 100% market share. • Application timing: all rails were sprayed at the same time step; relation of timing to specific dates did not apply as further simulation conditions (*e.g.*, wind direction) were also not dependent on specific dates; *i.e.*, no variability in application timing. • Application unit: individual railway (*e.g.*, Great Western Main Line).
Exposure	• Model: simple deterministic distance-dependent spray-drift deposition function; no variability of spray-drift deposition at equal distances from rails (*i.e.*, same deposition at same distance). • Spray-drift deposition depended on wind direction: deposition occurs downwind; *Exposure-Paths* (Section 5.3.5.3) represented potential wind directions; 8 potential wind directions of equal probability considered (compass directions N, NE, E, SE, S, W, SW); in each application run a random wind direction per railway was selected. • Superposition of spray-drift deposition into a single WB from different neighbouring rails was possible. • No switching-off of the application when crossing bridges over WBs as is done in reality, *i.e.*, the results contained a number of WB sections of unrealistic high exposure. • In an additional analysis step, spray-drift filtering due to riparian vegetation considered (PMF, Section 5.3.5.5); sampling of spray-drift filter effect by *Exposure-Path*.
EFate	• Instantaneous mixing of spray-drift deposition in WB segment represented by a receptor, according to the definitions of the Tier-1 scenario (WB depth = 0.3 m, static). • In case of multiple spray-drift depositions, exposure was added to substance residues already in the WB segment (receptor).

Entity	Definition
	• Dissipation of active substance not taken into account.
Effect	• Biological entity and attribute as represented in the Tier-1 ecotoxicological endpoint (NOAEC). • TER calculation; unacceptable effect indicated by TER<1.
Monte Carlo	• Monte Carlo (MC) approach with N=30 MC runs. • In each MC run, exposure and TER calculations for each receptor and time-step.
Risk Characterisation	• For aquatic plants, the (meta-) population was considered an appropriate biological entity, which relate to spatial extents. All WBs were assumed to be populated by the sensitive species which determined the ecotoxicological endpoint. • Risk was characterised in different scales. Two different ecological scales (units) were defined (i) WB_{pooled} – scale, (ii) $WB_{individual}$ – scale. • Ecological scales (units) were assessed in different spatial scales, defined as four different WB groups of WBs occurring within 1 km, 500 m, 200 m, 100 m from railways. • For each MC run (out of *N*) the distributions of exposure (PECsw) and effect (TER) over the receptors were evaluated by calculating location parameters (*e.g.*, 90th percentile PECsw = 'P90 PECsw'). These *N e.g.*, P90 PECsw built a distribution from which expectancy values were calculated, *e.g.*, <P90 PEC>. • At $WB_{individual}$ – scale, for each individual WB (and MC run), from the TERs of its receptors the fraction of the WB length was calculated that showed TER<1. From the *N* fractions, the probability of TER<1 was calculated for more than a given fraction of this WB. Again, these values build a distribution which was presented by percentiles and frequency distributions.

6.3.4.9 Spray-drift Filtering of Riparian Vegetation

Key results of the present landscape-scale risk characterisation were obtained without taking spray-drift filtering of riparian vegetation into account in order to keep the assessment conservative with respect to this potential risk mitigation factor. However, in a number of studies it was shown that riparian vegetation has the potential to significantly filter spray-drift by acting as a resistant to air movement and filtering droplets by leaves, branches, needles, twigs, etc. (Section 5.3.5.5). For demonstration purposes this potential filter effect was taken into account as obtained in a literature evaluation in an additional assessment (Section 5.3.5.5).

Natural streams and ecologically particularly viable ditches are typically accompanied by herbaceous riparian vegetation. As spatially explicit geodata on the occurrence of riparian vegetation was not available, general occurrence of herbaceous riparian vegetation was assumed for the intended demonstration purpose, and the spray-drift filter potential of this vegetation was applied as shown in Figure 37 (variability represented as PMF in Xplicit).

6.3.5 Results and Discussion

6.3.5.1 Spatial Analysis on Railway-to-Water body Co-occurrence

Risk of aquatic plant populations resulting from spray-drift deposition due to herbicidal product application on rails depend on local co-occurrence of application area (rails) and habitats (WBs). Significant exposure due to spray-drift is limited to the close vicinity of rails.

The analysis on the potential of railways to represent a significant source of spray-drift exposure revealed that the majority of railways have WBs in distances up to 1 km, which decreases to 29% of rails when focusing to 20 m distance (the 20 m threshold was used as an indicator for potential effects as up to about this distance the spray-drift deposition curve derived from the Tier-1 exposure calculation results in TER<1). Therefore, for distances relevant to RA drift about 29% of rails show significant potential to expose WBs.

Figure 68: Typical situation where WBs cross a railway. Their fraction close to rails is therefore small. Water bodies cross railways often in pipes underneath embankments.

Risk characterisation for aquatic plant (meta-) populations also focused on the individual WB. The fraction of WBs occurring in certain distances to rails was analysed, (i) for the entirety of WBs, and (ii) for each individual WB.

In up to 1 km from rails >30,000 km of WBs occur, whereas in distances up to 20 m, 644 km occur. Therefore, from all WBs occurring up to 1 km from rails (WB_{pooled}-scale), 2% of their length occur in an approximate distance at which spray-drift depositions can lead to TER<1. This estimation provides a first indication of potential risk of aquatic plant populations due to spray-drift of Herbicide-1 from rails in UK. Illustration of railway-to-WB co-occurrences are shown in Figure 68 and Figure 69.

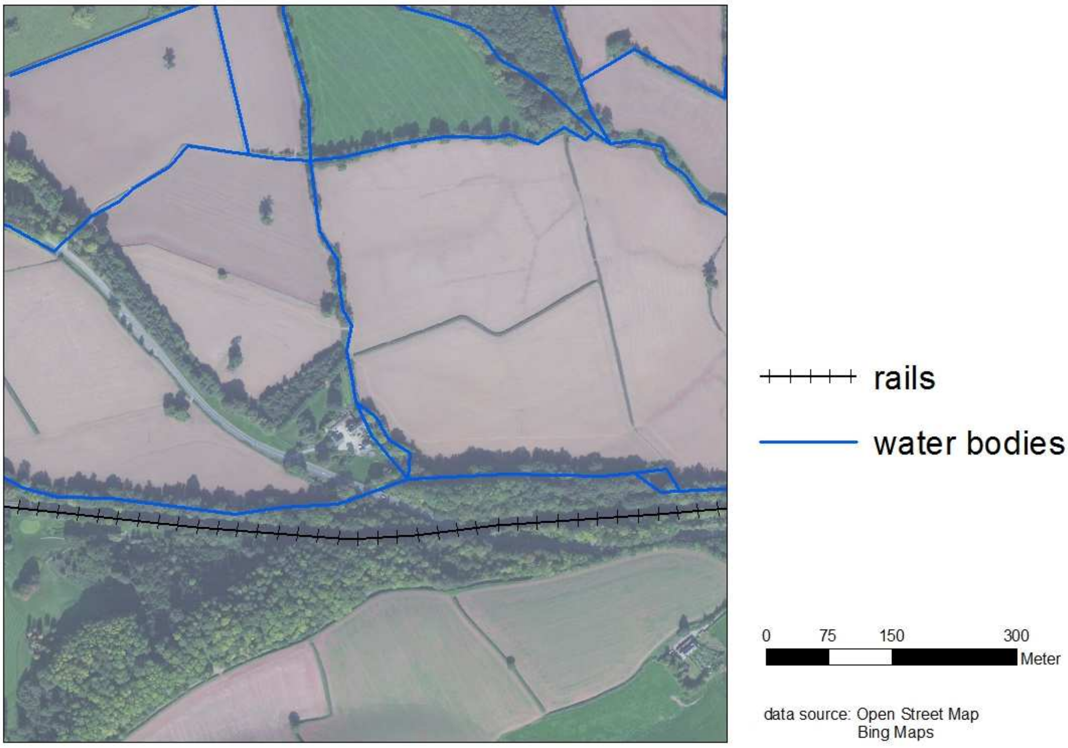


Figure 69: Example situation where a stream flows along rail for a certain length. The stream is accompanied by riparian vegetation and hardly gets closer than approximately 10 m.

The question whether local effects can aggregate in a few WBs was evaluated at the scale of individual WBs ($WB_{individual}$—scale). To this end, the fraction of individual WBs close to rails was calculated.

As shown in Figure 70, the majority of Water bodies in up to 1 km distance from railways are not closer than 20 m to rails (≈74%). Only about 26% of WBs occurring in up to 1 km distance from railways get that close to rails that significant effect due to spray-drift can occur. 94% of Water bodies in up to 1 km distance from railways have <10% of their length closer than 20 m to rails. Only 2% of WBs show fractions ≥50% of their length closer than 20 m to rails. Therefore, for the majority of WBs occurring in the vicinity of rails only a small portion of their individual sections occur in such vicinity to potentially receive significant spray-drift depositions. In other words: WBs usually do not flow along rails in very short distance, but rather cross the railway tracks. Therefore, only small parts are in close rail vicinity.

Focusing on WBs that are at least partly located within a 20 m distance from rails (*i.e.*, data of Figure 70, but excluding WBs of 0% fraction ≤20 m to rails, n = 6,233) showed that about 78% of WBs in ≤20 m distance to rails have <10% of their length closer than 20 m to rails.

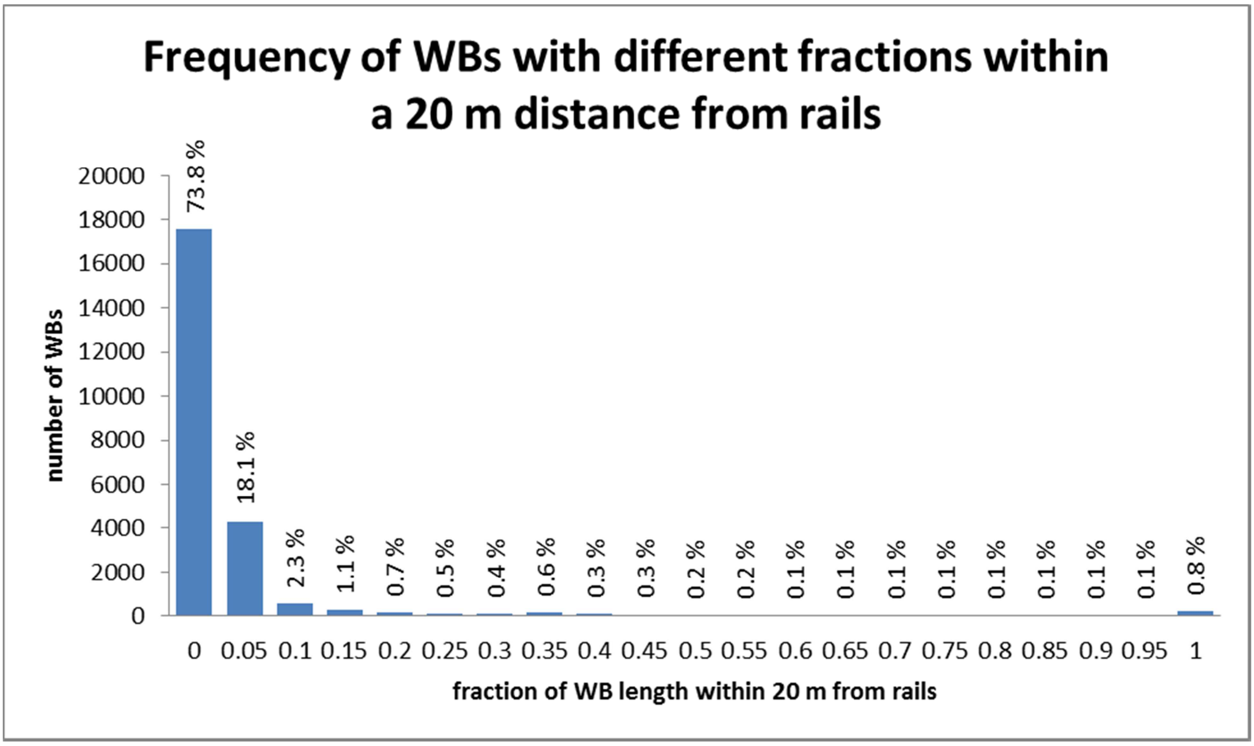


Figure 70: Fraction of individual WB length at ≤20 m distance from rails – all WBs occurring in a maximum distance of 1 km from rails (n = 23,794).

Assessment of these results should take into account that not entire streams are subject to this analysis but WB sections as represented in the OSM dataset. Such WBs sections are partly quite short and are artificial to a considerable part, *e.g.*, due to interruption of WBs by crossings, by multitrack railways or other man-made structures (Figure 72).

However, short WB sections partly also represent ditch sections occurring between agricultural fields and railways, whereas natural streams and ponds generally occur at considerable distance from rails (Figure 71). A visual inspection of railway-WB scenes revealed that rivers and streams that flow along railway tracks at large length are infrequently located in close vicinity. Especially (natural) streams are typically surrounded by a considerable riparian zone, that causes some naturally necessary distance to a man-made railway embankment (and can act as a filter for spray-drift, Figure 69).

Figure 71: Visual screening in GIS of short WB sections occurring in the vicinity or rails: *e.g.*, ditch sections in rail vicinity occurring between agricultural fields and railways (orange) and natural streams at considerable distance (green). Ponds typically occur in considerable distance to railways of which – as a conservative definition –only the shoreline was taken into account in the landscape-scale RA. (Remark: drift filtering due to riparian vegetation was not taken into account in main landscape-scale RA.)

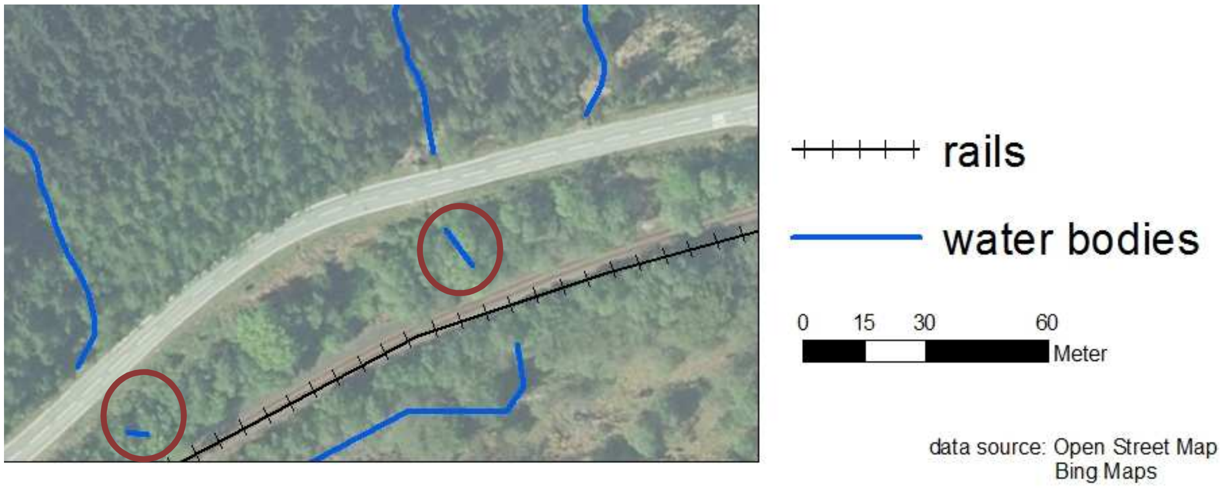


Figure 72: Short WB segments in the dataset (red circles) are often due to piping or locks, interrupting of their surface and representation in the geodataset.

6.3.5.2 Spatially Explicit Risk Characterisation

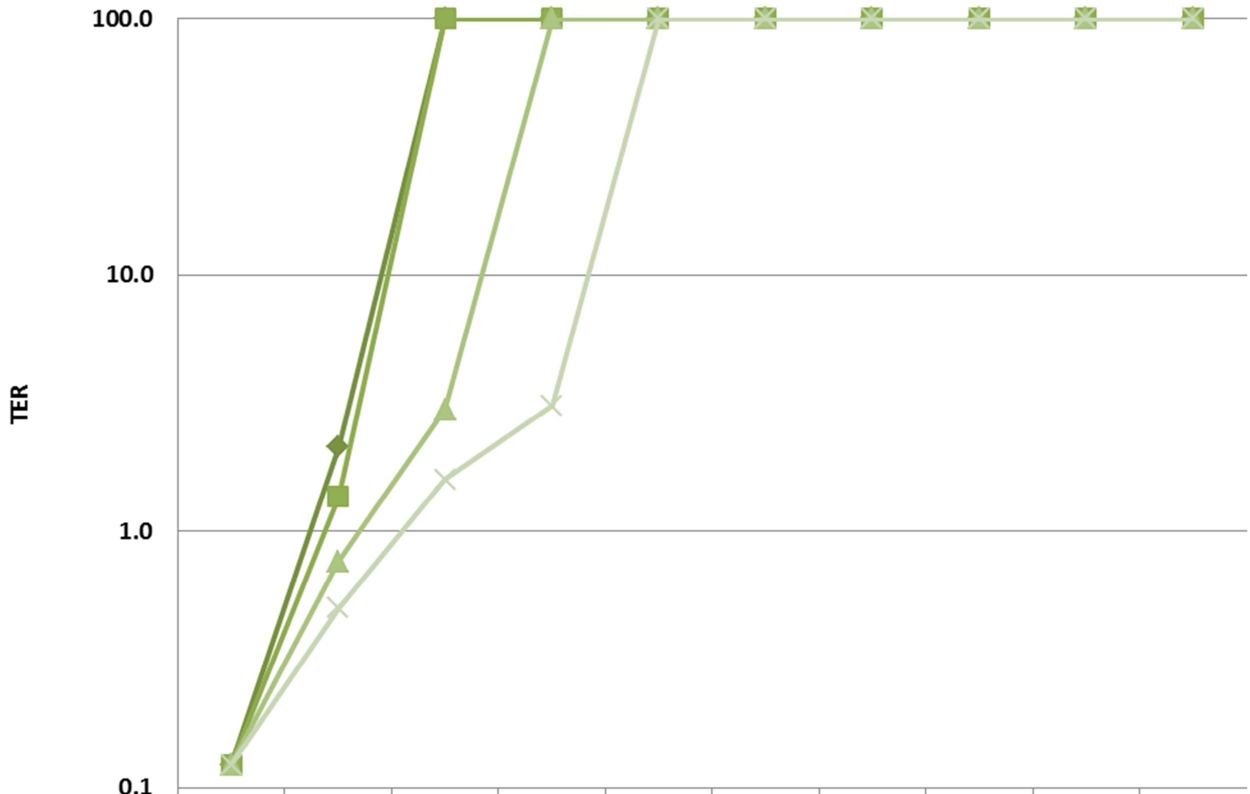
This section summarises the results of the *Xplicit-Rail-Model* simulations for the WB_{pooled}–scale and the $WB_{individual}$–scale. Results are presented for TERs, as resulting from the local PECsw and the ecotoxicological endpoint of Herbicide-1, for each of some 10^6 receptors (each representing a 5 m WB segment). Percentiles represent the expectancy values over the Monte Carlo runs. Switching-off of the application when crossing bridges over WBs, as done in reality, was conservatively not taken into account in the model approach, *i.e.*, the results contain a number of WB sections of high exposure which do not occur in reality.

WB_{pooled}-Scale

At WB_{pooled}-scale, all WBs occurring in the vicinity of rails built a single 'set'. Four WB groups built the basis of the analysis, distinguished by their maximum distance from rails: 1 km, 500 m, 200 m, 100 m.

Results are summarised in Figure 73, showing percentiles of the cumulative distribution of TERs for the 5 m WB segments (receptors) by spatial group. As the results demonstrate, the large majority of WB segments are unlikely to receive spray-drift depositions from the use of Herbicide-1 on rails in UK that result in a TER<1: *e.g.*, for 90% of the WB segments the TER is >100 for the 1 km, 500 m and 200 m WB group; for <1% of the WB segments the TER of 1 can be violated (*e.g.*, for <1% of WB segments the TER≤0.76 for the 200 m group); for 90% of WB segments TER is >3.1 for 100 m WB group. The minimum TER obtained in the landscape-scale RA was below the Tier-1 value, which is due to superposition of exposure from multiple rails in vicinity of a WB segment.

In summary, for the majority of WB segments occurring in the vicinity of rails the TER is >100 indicating that unacceptable effects are not likely to occur at large spatial extent.



	min	P1	P5	P10	P20	P50	P75	P90	P95	max
1000m	0.12	2.13	100	100	100	100	100	100	100	100
500m	0.12	1.36	100	100	100	100	100	100	100	100
200m	0.12	0.76	2.99	100	100	100	100	100	100	100
100m	0.12	0.50	1.60	3.10	100	100	100	100	100	100

Figure 73: TER [no unit] distribution by WB group (calculated TERs >100 were set to 100, Px = xth percentile) - WB_{pooled}-scale.

This assessment was supported by visual inspection of rails-to-WB co-occurrences and TER distributions of WB segments in GIS. Maps on the spatial distribution of PECsw and TER violations are shown in Figure 74 to Figure 76. As the maps indicate, only a small fraction of WB sections occur close to railways. Close vicinity mainly occurs in case a WB crosses a railway. In this situation, only limited fractions of an individual WB can receive significant spray-drift deposition. Spray-drift filtering of riparian vegetation was not taken into account in the calculations for refined RA (only for demonstrative purposes, below).

Figure 74: Spatial distribution of PECsw for riparian water zone of ponds and small lakes (1 MC run). Railway running from north-west to south-east; western wind direction; dots indicate WB segments in ≤50 m distance to rails; spray-drift filtering by riparian vegetation not taken into account (green dots: TER≥1). No TER = 1 violation due to considerable rail-to-WB distance.

Figure 75: Larger natural stream meandering through an agricultural landscape. Railway running from south-west to north-east (black line). Spatial distribution of PECsw (1 MC run); north-western wind direction; dots indicate WB segments in ≤50 m distance to rails; spray-drift filtering by riparian vegetation not taken into account; red dots: TER<1, green: TER≥1). Few local WB segments of TER<1.

Figure 76: Spatial distribution of PECsw of WBs (1 MC run) in up to 1 km distance from rails in agricultural area (blue, predominately ditches, some streams). Two railways which meet at the northern centre of the image; western wind direction; dots indicate WB segments in ≤50 m distance to rails; spray-drift filtering by riparian vegetation not taken into account (red dots: TER<1, green: TER≥1). Few local WB segments of TER<1, mostly at locations where railway crosses. Therefore, TER<1 WB sections are mostly of limited length.

$WB_{individual}$-Scale

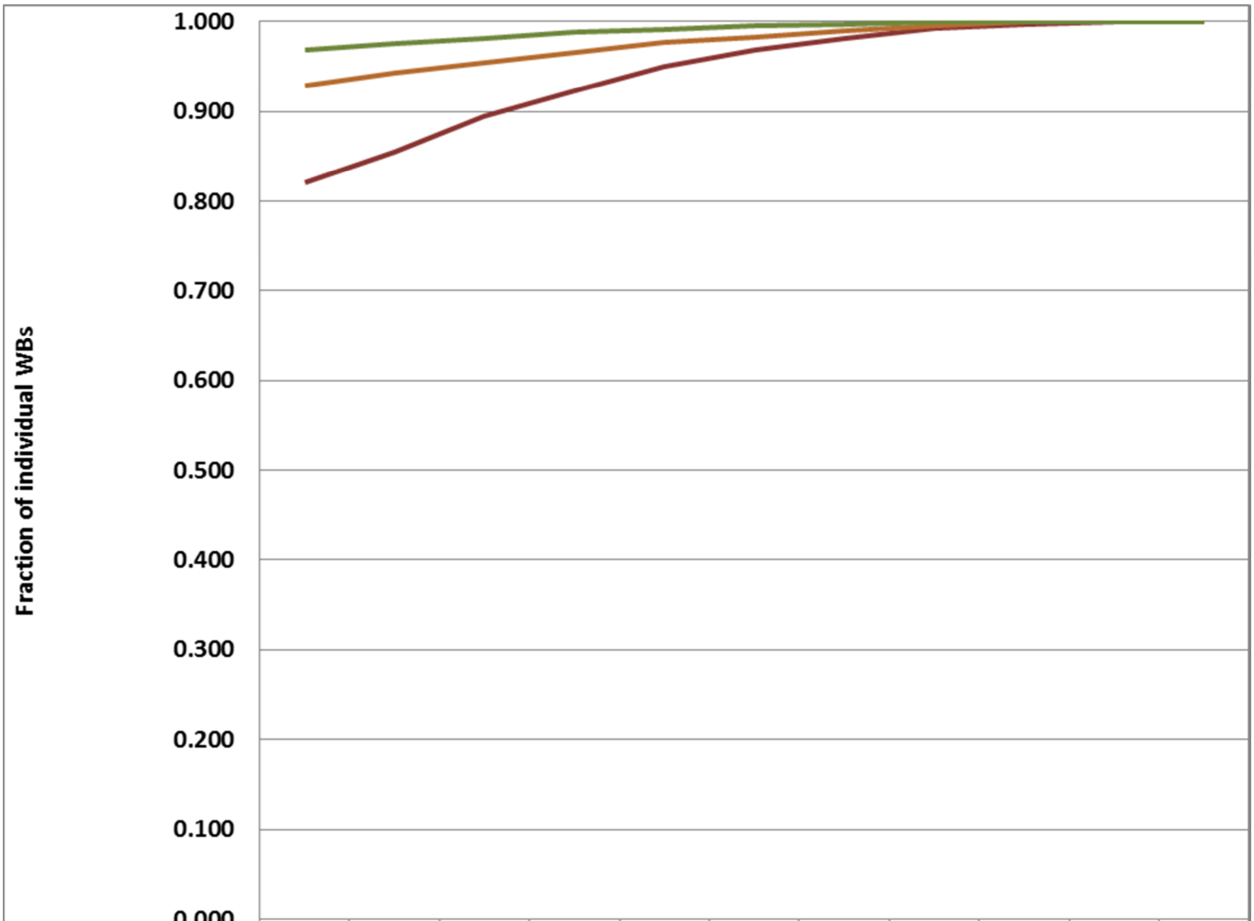
This section summarises results of the *Xplicit-Rail-Model* simulations obtained for each individual WB ($WB_{individual}$-scale). This analysis addresses the question to which extent high exposure values (PECsw), and hence, TER of 1 violations, can aggregate in individual WBs.

There is a large number of WBs which occur in up to 1 km from rails, yet, not very close to railways (above). In order to focus on WBs that can actually show an aggregation potential, this analysis was focused on WBs which occur in the 100 m WB group. This also is a clearly defined and consistent context to assess risk acceptability.

Results are presented in Figure 77. The graph shows the cumulative fraction of individual WBs (ordinate) by the probability of TER<1 occurrence (abscissa) for certain WB fractions (>10%, >20%, >50%): *e.g.*, 0.821 (82.1%) of individual WBs, occurring at least partly in a maximum distance of 100 m to railways, have a probability of zero (P=0) that the a TER<1 will occur for more than 10% of their length; for 0.975 (97.5%) of individual WBs the probability is less than 0.1 (10%) that more than 50% of their length show TER<1. Results were obtained without taking spray-drift filtering by riparian vegetation into account.

Absolute numbers of WBs of higher probability to violate the TER trigger at considerable extent can be calculated by multiplying the total number of WBs occurring in the WB set defined above (n=9,069) with the resulting fraction: *e.g.*, about 0.5% (1-0.995) of all WBs occurring in up to 100 m distance have a considerable probability of P>0.5 (50%) of TER<1 for >50% of their length ($P_{(TER<1,\ fraction>50\%)}$>0.5); thus, in total, in entire UK around 45 WBs are expected to show such conditions (9069 · 0.5%). A probability of 0.5 (50%) can statistically be interpreted that this event of TER<1 for >50% of the WB length can happen every other year (for 45 WBs in total). A subset of such WBs was undertaken a closer evaluation in the GIS: none of such WBs could be recognised as a natural stream. High $P_{(TER<1)}$ is partly an artefact of (very) short WB segments in the geodata due to interruption by pipes, weirs, small WB sections that occur between multitrack railways, etc., yet, was partly obtained for (short) drainage ditches occurring between an arable field and the railway.

In case RA of individual WBs results in unacceptable risk, risk characterisation at $WB_{individual}$-scale can be directly introduced in RM: the geographic locations (coordinates) of potentially vulnerable WBs could be used to, *e.g.*, locally adapt the herbicidal use rate (up to switching-off) or to design a generic RM campaign (*e.g.*, adaptation of WB maintenance).



	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
fraction >10%	0.821	0.854	0.894	0.924	0.950	0.968	0.981	0.992	0.997	0.999	1.000
fraction >20%	0.929	0.942	0.954	0.966	0.976	0.983	0.990	0.996	0.999	1.000	1.000
fraction >50%	0.968	0.975	0.981	0.988	0.991	0.995	0.997	0.999	1.000	1.000	1.000

Figure 77: Cumulative portion of individual WBs occurring at least partly in a maximum distance of 100 m to railways (ordinate) by probability (abscissa) of TER<1 for certain WB fractions (>10%, >20%, >50%).

6.3.5.3 Effect of Limitations in the Representation of Water Bodies in Geodata

As described in Section 6.3.4, the representation of WBs in the geodata was inspected. For a subset of railways (13 railways of a total length of 1,524 km), representation of WBs in the dataset was corrected (or added by digitisation). The corrected dataset was compared with the original geodata, by *Xplicit-Rail-Model* simulations as applied in the full analysis (WB_{pooled}–scale).

In summary, the occurrence of WBs in the original dataset was confirmed. Especially, natural stream were well presented. For the 1 km and 500 m WB group no differences were obtained for the RA between the original and the corrected dataset. For the 90th percentile PECsw, impacts on exposure assessment were only detectable for the 100 m WB group. For this WB group the manually processed geodata increased the 90th percentile PECsw by approximately

12.5%. The maximum PECsw was not affected. Therefore, the UK-wide WB dataset used in the main investigation (above) was regarded appropriate to characterise risk of aquatic plants due to spray-drift of a herbicidal product when used on rails in UK.

6.3.5.4 Effect of Spray-drift Filtering by Riparian Vegetation

Natural WBs are typically accompanied by riparian vegetation. For demonstration purposes, *Xplicit-Rail-Model* simulations were conducted on WB_{pooled}-scale assuming that WBs are accompanied by grass of herbaceous vegetation.

In summary, the calculations resulted in exposure reductions of more than 60% at WB_{pooled}-scale (100 m WB group). Spray-drift filtering by riparian vegetation can contribute to local variability of exposure as the filter effect can vary at local scale. The filter effect is likely to reduce the probability of local TER violation to occur at larger WB length at $WB_{individual}$-scale.

6.3.6 Conclusions

Characterisation of risk of aquatic plants due to spray-drift depositions of herbicidal products into WBs adjacent to railways can be significantly improved by defining a landscape-scale approach related to SPGs.

A straightforward spatial analysis (GIS) provided a first indication that potential exposure of WBs due to spray-drift from rails is limited to small fractions of the entire WB set and also of individual WBs' length. These results were consistent with the detailed spatiotemporally explicit and probabilistic analysis obtained using the *Xplicit-Rail-Model* (below).

At WB_{pooled} – scale, *i.e.*, assessing the entirety of WBs without distinguishing individual WBs, the vast majority of WB segments are unlikely to receive spray-drift depositions that result in a TER<1: *e.g.*, TER<1 was obtained for <<1% of WB segments in 1 km WB group (<5%, 100 m WB group). At $WB_{individual}$ – scale, *i.e.*, explicit RA for each individual WB, it was found that high exposure values (leading to TER<1) occurring at large extent of an individual WB are rare. Thus, aggregation of effects in individual WBs is infrequent. This is first of all as typically WBs only occur with small fractions of their length close to railways (*e.g.*, intersecting rails) and as natural WBs (*e.g.*, streams, ponds) apparently mainly occur at considerable distances.

A few WBs (<1% of WBs occurring in up to 100 m from railways) were indicated to show higher probability of TER<1 at large extent of their length. By screening the geodata, these were found to be either artefacts (*e.g.*, small WB sections between multitrack railway bridges) or ditch sections occurring between agricultural fields and railways. For the majority of WBs occurring in the vicinity of rails the TER is >100 indicating that unacceptable effects are not likely to occur at large WB extent, hence, plant (meta-) population extent. This applies to the entirety of the WB network in the surrounding of rails, as well as to the large majority of individual WBs.

Limitations in the representation of WBs in the geodata employed are not expected to significantly change the key results, nor the conclusions on risk characterisation.

Therefore, the entirety of the results of the present study suggest that risk to aquatic plants due to spray-drift from the use of herbicidal products on rails appears limited. This is supported by the fact that herbicidal use on railways are infrequent (typically one per season) which facilitates recovery of plants from potential local effects.

This conclusion contains additional safety margins, as the study results were derived on different conservative definitions, *e.g.*, 100% rails are treated with Herbicide-1, all rails were assumed double track with both tracks assumed to be sprayed at the same time, no riparian vegetation or other natural drift mitigating factors present and the fact that switching-off of the application when crossing bridges over WBs was not taken into account.

In case RA of individual WBs indicates high vulnerability, risk characterisation at $WB_{individual}$-scale can be directly used in RM: the geographic locations (coordinates) of potentially vulnerable WBs could be used to, *e.g.*, locally adapt the herbicidal use rate (up to switching-off) or by conducting a generic RM campaign (*e.g.*, adaptation of WB maintenance).

The study results provide a significant improvement in risk characterisation compared to the standard Tier-1 level and are regarded sufficiently robust to support RM decision-making.

Future developments are suggested to consider means of mechanistic (meta-) population modelling to assess ecological effects at actual protection goal level of aquatic plants (ecological modelling, Section 5.3.5.7). Hydrological modelling can increase realism of eFate characterisation and, together with geodata on surrounding land use, can provide a step towards increased *SynContext* (Section 4.1) in ecological RA and RM. In this context, the Xplicit approach can support the development of ecological scenarios (Reference Scenarios, EFSA 2010a, Section 4.3.2).

The study provides information on risk of different WB types, and shows that risk of artificial manmade ditches is higher than that of natural streams. Thus, risk of ditches can determine RM measures which can have a significant impact on railway maintenance options. Therefore, and provided that sufficient knowledge on risk is available, different protection levels distinguished by WB type might be considered.

Still, the use of geodata from public institutions is hampered by restrictive pricing and licence policy. A concerted panel is proposed to discuss future options of public data access policies.

Risk characterisation as shown in this study involves a range of disciplines, working at the aim to provide a sound basis for adequate and effective RM. Besides good science, this process requires good risk communication at a number of levels along the process. As this is not a core discipline of scientists, adapted trainings might be considered (*e.g.*, SETAC 2013a).

6.4 Risk Characterisation for Aquatic Organisms in North Rhine-Westphalia, Germany

This case study was intended as a pilot study to explore the use of small-scale topographic geodata in refined risk characterisation for large regions using the Xplicit approach. Different key aspects related to refined risk characterisation were explored (*e.g.*, comparison to the Tier-1 scenario, effect of RM, data improvement, population-level RA).

6.4.1 Lessons Learned

- The spatiotemporally explicit and probabilistic approach allows to assess risk as defined in Section 4.3.1. Consideration of scale dependencies is key to risk characterisation.
- The Xplicit approach can provide a sound basis to determine adequate RM measures at large spatial extent (up to entire Germany). Aggregation potential of high risk segments ('Hot-Spot') can be assessed at ecologically relevant scales. General design options for RM can contribute to balance ecological and economic requirements. Strategies for specific RM design can be evaluated, *e.g.*, maintaining strategy of riparian vegetation as a filter for spray-drift based on scale-dependent variability analysis.
- Safety margins built into current lower-tier RA levels can be quantified. Such analysis can build a basis to define future lower- or reference-Tier scenarios (*e.g.*, EFSA 2010a) with predefined safety margins.
- With its modular approach, *Xplicit-Models* can identify main drivers of risk or RM, and so, can identify research needs, *e.g.*, to improve data or process modelling.
- *Xplicit-Models* can operate with mechanistic ecological models. Initial steps were undertaken to introduce PECsw into a (meta-) population model for the 'waterlouse' *Asellus aquaticus* (MASTEP, van den Brink *et al.* 2007, Galic 2012).

6.4.2 Abstract

Spray-drift deposition is an major potential entry route of PPPs into water bodies occurring in vicinity to fields. Exposure of aquatic organisms due to spray-drift was estimated at landscape-scale using an *Xplicit-Aquatic-Model* on the basis of readily available topographic geodata (ATKIS).

The study was designed as a pilot study to explore the following goals: (i) estimation of the distribution of potential exposure due to spray-drift at landscape-scale for a large regional extent (State 'North Rhine-Westphalia', NRW, Germany), and comparison to the Tier-1 scenario, (ii) comparison of the efficiency of RM measures, (iii) gain of technical experience in operating large datasets, and (iv) provision of a proposal on the future use of medium-scale topographic data (*e.g.*, ATKIS) in landscape-scale risk characterisation.

A crop protection measure was assumed to be conducted at 90% of all arable fields occurring in the vicinity to water bodies in NRW, within a week's time period. The PPP was applied once at 100 g a.s./ha. The a.s. was fast-dissipating in the aquatic phase (DT50 = 1 day). An aquatic Assessment Endpoint of 0.1 µg/L was assumed. At standard Tier-1 RA level, a TER = 0.1 was

obtained. Assuming a 10 m buffer (no-spray) zone, the Tier-1 TER increased to about 1.0, which was regarded to indicate acceptable risk.

At landscape-scale, ATKIS data showed ≈17,000 km of linear water bodies occurring in a maximum distance of 1 km of arable fields (≈2,900 water bodies). This includes the conservative assumption that water bodies occurring remote from arable fields were not relevant for ecological risk characterisation. Distant-dependent spray-drift deposition variability was modelled using the empirical model of Golla *et al.* (2011) and assuming even distribution of wind directions. As RM options, drift reducing application technology, buffer (no-spray) zones (5 m, 10 m), and spray-drift filtering by riparian vegetation were assessed. WB characteristics were kept as defined in the Tier-1 scenario.

Spatiotemporally explicit exposure and effect simulation was conducted using an *Xplicit-Aquatic-Model*, which was derived from the *Xplicit-Framework*. Water bodies were discretised into 5 m segments. Outcome was assessed, (i) by pooling all water bodies (WB_{pooled} - scale), and (ii) for each individual WB ($WB_{individual}$ – scale). RA was mainly based on 90th percentile exposure, representing an agreed realistic worst-case in RA.

At WB_{pooled} – scale, without filter effect of riparian vegetation, the same RM combinations of drift reducing technology and buffer zones are required to achieve acceptable risk as at Tier-1. This result does not depend on positional accuracy of small-scale geodata because in intense arable cultivations especially drainage ditches occur in close vicinity to fields. This conclusion depends on the protection level of small manmade drainage ditches and can change in case protection goals of ditches are regarded lower than that of natural streams. When taking filter effect of riparian vegetation into account, RM requirements regarding drift reducing technology buffer zone are lower than at Tier-1. Then, either 50% drift reducing technology, or 5 m buffer could represent a sufficient protection level.

The indicated importance of riparian vegetation as RM is suggested to be further substantiated by more systematically generating data on filter effects of (riparian) vegetation in dependence of agricultural and environmental conditions. This data generation should be done in relation to geodata improvement, to which an iterative enhancement cycle is proposed.

$WB_{individual}$ – scale addresses an ecologically relevant scale for RA and RM ('Hot-Spots'). The analysis demonstrates the strength of the Xplicit approach in assessing scale-dependent probabilities of quality criteria violations. RM measures leading to risk acceptability at WB_{pooled} – scale reduced the probability *Pvio* PECsw > 0.1 µg/L for >10% of individual WB length to *Pvio* = 0 for ≈100% of water bodies. Meeting the assessment criteria at WB_{pooled} – scale is a necessary precondition to meet the criteria at $WB_{individual}$ – scale, but is not sufficient, as theoretically violations could aggregate in a view water bodies. Discrete RM measures can significantly reduce risk of individual water bodies. In the example, risk disappears when a 50% drift reduction or a 5 m buffer zone were imposed in addition to existing filter vegetation. Reversely, having defined risk acceptability criteria, appropriate RM measures can be identified to balance ecological risk with economic cost.

The *Xplicit-Framework* is capable to process large landscapes. Calculation time of this study indicates that processing all water bodies in Germany (192,000 km in the vicinity of arable fields) should be possible.

The spatiotemporally explicit exposure estimation ($PEC_{(r,t)}$) provided by the *Xplicit-Aquatic-Model* are prepared to be used as input for a population model for aquatic invertebrates (MASTEP) in order to characterise risk at population level.

6.4.3 Introduction & Objectives

Spray-drift deposition is a major potential entry route of PPPs into water bodies occurring in vicinity to fields. RA for aquatic Non-Target-Organisms due to spray-drift is based on the standard Tier-1 aquatic exposure assessment. This scenario assumes a shallow (30 cm deep) ditch of static water, located downwind, in 1 m distance to a treated field. Spray-drift depositions are assumed to reach the water surface of the ditch as depositions reached the ground level in spray-drift deposition measurements (Ganzelmeier *et al.* 1995, Rautmann *et al.* 2001), as the water level of the ditch is assumed at ground level (no shielding due to profile geometry). The ditch is further assumed without riparian vegetation which can act as spray-drift filter. From the range of spray-drift depositions measured in empirical studies (Rautmann *et al.* 2001), the 90th percentile is assumed to deposit on the water surface.

In case the Tier-1 RA indicates unacceptable risk for a specific PPP, mitigation measures can be imposed to the PPP use (product label), which typically comprise the use of spray-drift reducing application technology and imposing a buffer zone, *i.e.*, a minimum distance the farmer has to keep between sprayer and WB for the use of the PPP.

Besides PPP specific risk mitigation, generic RM measures can provide effective means to reduce spray-drift entries into water bodies for all PPP uses: *e.g.*, generic no-cropping zone, maintenance of good status of riparian vegetation that can act as a filter for spray-drift (Section 5.3.5.5), constructed wetlands for substance retention, etc. Effects of such measures are generally also in good agreement with further environmental protection goals (Section 4.3). With efficient generic RM measures PPP-specific risk mitigation measures could be optimised from economic and ecological perspectives. The potential of generic RM in relation to PPP-specific mitigation measures was investigated in different projects (*e.g.*, GeoPERA project of the German Crop Protection Association, IVA, Schad *et al.* 2006b, 2007, Schad 2006a at SETAC GLB Landau, GeoRISK, UBA, FKZ 3707 63 4001, Schulz *et al.* 2007, 2009). Besides regulatory problems between PPP-specific authorisation and generic RM regulations, the projects revealed different methodological problems. Among these were, *e.g.*, basic questions on how to design probabilistic exposure assessment (*e.g.,* take scale-dependencies in a Monte Carlo approach), in order to assess statistically independent cases that represent realistic pattern. Also, the representation of water bodies and their spatial relationship to fields in adequate resolution were of concern.

With respect to protection goals (Section 4.3.2), risk is to be characterised at (meta-) population level. This requires to propagate individual level effect to (meta-) population effect, which can be done by means of ecological modelling (Section 5.3.5.7).

In this context, the presented pilot study had the following objectives:

i. Estimation of the distribution of potential exposure due to spray-drift at landscape-scale for a large regional extent (State 'North Rhine-Westphalia', NRW, Germany) and comparison to the Tier-1 scenario. To this end, readily available topographic geodata

(ATKIS) were used and variability of local spray-drift depositions and wind directions were taken into account. In doing so, refinements to risk characterisation are mainly due to landscape composition and structure. This should provide a first impression on the distribution of potential exposure due to spray-drift at two landscape-scales, (a) the entirety of WB segments as a single set (WB_{pooled} – scale), and (b) by individual WB ($WB_{individual}$ – scale). The $WB_{individual}$ – scale is in particular focus of the analysis as it represents an ecologically relevant scale for local RM ('Hot-Spot' management).

ii. Relative comparison of efficiency of different RM measures at landscape-scale, comprising drift-reducing application technology, buffer (no-spray) zones, and the occurrence of riparian vegetation as spray-drift filter.

iii. Gain experience in operating large datasets in Xplicit.

iv. Provide a proposal on the use of medium-scale topographic data (*e.g.*, ATKIS) in combination with an iterative sampling approach to locally enhance geodata using high-resolution remote sensing imagery.

v. Preliminary link of Xplicit with an *Individual-Based-Model* (MASTEP) to assess ecological effects at (meta-) population level.

Natural variability of WB conditions, weather and further environmental and agricultural conditions, as well as limitations in the representation of entities in geodata, impose clear limitations to the predictive power of landscape-scale risk characterisation at different scales. This is reflected in the study goals which essentially take the Tier-1 scenario as starting point.

6.4.4 Data & Methods

6.4.4.1 GeoData

Characterisation of land use/cover of NRW, Germany, was based on the topographic geodata ATKIS (Authoritative Topographic-Cartographic Information System, Figure 78) which is a product of the Cadastral and Surveying Authorities who are responsible for the Official German Surveying and Mapping (AdV 2012). ATKIS is of an estimated map scale of 1:25,000. This medium-scale geodata comes with generalisations in the spatial and thematic representation of entities which affect the scope of landscape-scale risk characterisation studies. In this respect empirical evidence were gained in joint projects of research, authorities and industry showing that natural streams and larger water bodies are well represented in ATKIS (GeoPERA project of the German Crop Protection Association, IVA, Schad *et al.* 2006b, 2007, Schad 2006a at SETAC GLB Landau; GeoRISK, UBA, FKZ 3707 63 4001, Schulz *et al.* 2007, 2009). Representation of smaller (drainage) ditches is heterogeneous across German States, yet, is beyond the cartographic requirements of ATKIS. From experiences gained in projects above (drainage) ditches are largely represented in ATKIS. As manmade and often quite intensively maintained structures, protection goals of (drainage) ditches need closer examination in the context of SPGs (EFSA 2010a). The study was focused on water bodies which are related to arable cultivation areas in order to avoid 'dilution' of the RA and RM conclusions by habitats of lower ecological relationship. Therefore, only water bodies in up to 1 km distance from arable were taken into account.

ATKIS represents land use units with the consequence that neighbouring individual fields of the same land use type (according to ATKIS) are generally represented as single geometric polygons. In the present study, this has the main consequence that in the spatiotemporally explicit model, applications of farmers were conducted on larger spatial units than the actual fields, which means that local temporal variability of exposure is aggregated to a single time-step event. With respect to the study goals, this can be regarded as conservative, as it potentially results in over-prediction of local WB exposure at single time-steps.

Regarding local exposure modelling (in scales between 10^0-10^1 m), a more critical issue of ATKIS is that local spatial relationships of approximately <10^1 m are rarely resolved (according to experience from joint projects, above). This affects the scope of landscape-scale studies, as it leads to systematic and significant over-prediction of local exposure compared to results obtained on the basis of high-resolution geodata (map scale ≈1:5,000, Schad 2006a, Schad *et al.* 2007). As ATKIS is currently the best available base geodata to cover entire Germany, methods to enhance ATKIS were examined. In the present study, given limitations led to the following steps: (i) use of a minimum crop-to-WB distance of 1 m (Rautmann *et al.* 2001), (ii) development of a proposal for a sampling method to enhance of ATKIS for landscape-scale aquatic RA and RM ('ATKIS^{+}', Section 6.4.3).

Riparian vegetation is generally not represented in ATKIS (ATKIS holds some related types, *e.g.*, hedges etc., yet, experience has shown that the quality of consistent representation is underdeveloped). Experience gained in the above mentioned projects (including field observations and expert judgement) consistently shows that especially natural streams are typically accompanied by riparian vegetation. Basically, this applies also to manmade drainage ditches. Herbaceous, and especially high riparian vegetation (*e.g.*, hedges, bushes, trees) can significantly filter spray-drift (Section 5.3.5.5). In the examination of the effect of riparian vegetation as a RM option, the occurrence of herbaceous ('low') riparian vegetation was assumed around linear water bodies.

All arable land use indicated by ATKIS was assumed the target crop for the PPP use. Future refinements may include regional cropping statistics (*e.g.*, 'Agrarstrukturerhebung' in Germany, DStatis 2013) to define actual field crops and to consider crop rotation.

Geodata taken from ATKIS were analysed by means of GIS software (ArcGIS version 10, ESRI 2012) in order to quantify the co-occurrence of arable and water bodies. This straightforward spatial analysis provided a first indication on the potential aquatic risk and served for consistency check for spatiotemporally explicit risk characterisation.

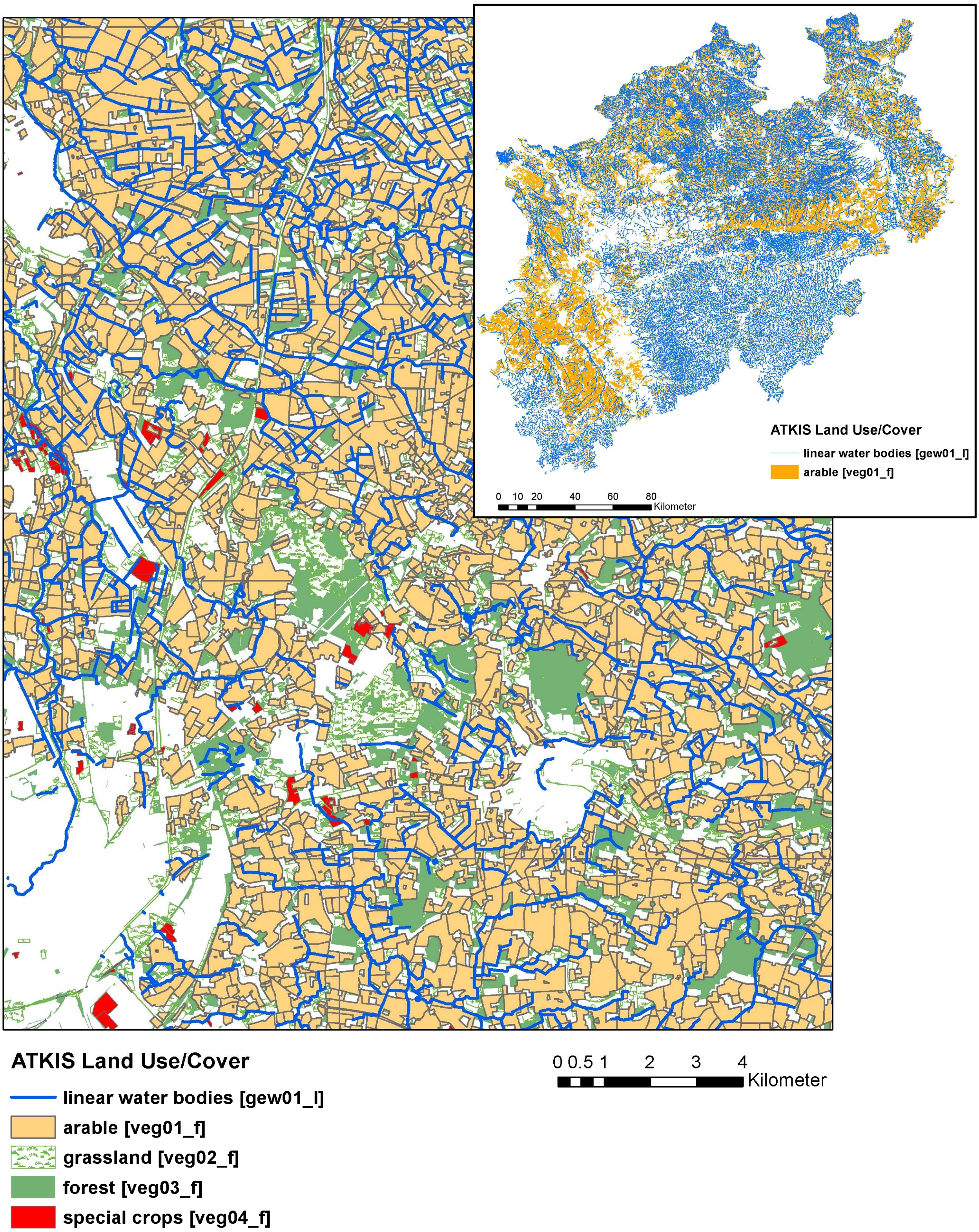


Figure 78: Excerpt of ATKIS data for NRW, Germany.

6.4.4.2 Xplicit-Aquatic-Model

Spatiotemporally explicit exposure and effect assessment was done using an *Xplicit-Aquatic-Model*, which was derived from the *Xplicit-Framework* (Section 5). The definitions of the *Xplicit-Aquatic-Model* are summarised in Table 23.

Table 23: Definitions of the *Xplicit-Aquatic-Model* (WB=water body).

Entity	**Definition**
Key study entities	PPP application areas (arable fields), WBs, individuals and (meta-) populations of aquatic invertebrates.
Landscape geodata	Topographic geodata (ATKIS) for NRW ('North Rhine-Westphalia', Germany) representing arable fields (≈1.2 Mio ha) and linear WBs occurring in arable cultivations (≈2,900 WBs of ≈17,000 km length occurring in a maximum distance of 1 km of arable fields).
Receptors	• WB segments of 5 m length, representing habitats of Non-Target-Organisms; discretised from WBs which were represented by lines. • WB definitions kept as in Tier-1 scenario (*e.g.*, WB depth = 0.3 m).
PPP use (Farmer)	A crop protection measure was assumed to be conducted at 90% of all arable fields occurring in the vicinity to water bodies in NRW, within a one week time period. The PPP was applied once at 100 g a.s./ha.
Exposure	• Probabilistic, distance-dependent spray-drift deposition (Golla *et al.* 2011). Minimum field-to-WB distance of 1 m. • Spray-drift deposition depended wind direction: deposition occurred downwind; *Exposure-Paths* represented potential wind directions; 8 potential wind directions of equal probability considered (compass directions N, NE, E, SE, S, W, SW); for each application a random wind direction per field was selected. • Spray-drift depositions reached the WB surface as assumed in the Tier-1 scenario, *e.g.*, no interception due to WB geometry. • Superposition of spray-drift deposition into individual WB segments (receptors) from different neighbouring fields could happen. • Depending on the defined RM option, buffer zones were taken into account (5 m, 10 m). • Depending on the defined RM option, spray-drift reducing application technology was taken into account. For the sake of simplicity and to keep in the official schemes, the effect of drift-reducing technology (nozzles) was deterministically taken into account (50% reduction). • Depending on the defined RM option, spray-drift filtering due to riparian vegetation was considered (PMF, Section 5.3.5.5); scale-dependent sampling of spray-drift filter effect (*Exposure-Path*, field).
EFate	• Instantaneous mixing of spray-drift depositions in WB segment

Entity	Definition
	(receptor), according to the definitions of the Tier-1 scenario (*e.g.*, WB depth = 0.3 m, static). • In case of multiple spray-drift depositions, exposure was added to residues already in the WB segment (receptor) within time-steps. • Fast-dissipating substance in the aquatic phase (DT50 = 1 day).
Effect	• An aquatic Assessment Endpoint of 0.1 µg/L (most sensitive species) was assumed in TER calculations (Assessment Factor = 1). • Remark: At standard Tier-1 assessment level, a TER = 0.1 was obtained without mitigation measures. Assuming a 10 m buffer (no-spray) zone, the Tier-1 TER increases to about 1.0, indicating acceptable risk.
Monte Carlo	• Monte Carlo (MC) approach with N=30 MC runs. • In each MC run for each receptor exposure and TER were calculated.
Risk Characterisation	• Expectancy values for percentiles of PECsw and TER. • Risk was characterised in different scales. Two different ecologically relevant scales were defined (i) all WBs occurring in arable cultivations pooled in a single unit (WB_{pooled} – scale), (ii) all individual WBs occurring in arable cultivations, *i.e.*, risk distinguished by WB ($WB_{individual}$ – scale). WB_{pooled} – scale sees the WB network as a whole independent of whether individual sections are connected or not, whereas $WB_{individual}$ – scale resolves individual connectivity. • For each MC run (out of *N*) the distributions of exposure (PECsw) and effect (TER) over the receptors (>3 Mio.) were evaluated by calculating location parameters (*e.g.*, 90th percentile PECsw, P90 PECsw). These *N e.g.*, P90 PECsw built a distribution from which expectancy values were calculated. • For each individual WB ($WB_{individual}$ – scale) and MC run, from the PECsw (TERs) of its receptors, the fraction of the WB length was calculated that showed PECsw>$trigger_1$ (TER<$trigger_2$). From the *N* fractions, the probability was calculated that a trigger would be violated for more than a given fraction of the individual WB.

6.4.4.3 Spray-drift Filtering of Riparian Vegetation

In a number of studies (Section 5.3.5.5) it was quantitatively shown that riparian vegetation has the potential to significantly filter spray-drift by acting as a resistant to air movement and filtering droplets by leaves, branches, needles, twigs, etc. This filter effect was taken into account in *Xplicit-Aquatic-Model* scenarios, in order to assess its potential as a RM option (Table 24). Naturally, filter effect can vary at local scale (10^0-10^1 m), *e.g.*, due to varying vegetation conditions (height, density, width, etc.). Yet, filter variation can also be related to local agricultural and maintenance conditions. Therefore, variability of spray-drift can be assigned to *Exposure-Path-* or field-scale.

Natural streams and ecologically particularly viable ditches are typically accompanied by herbaceous riparian vegetation. As spatially explicit geodata on the occurrence of riparian vegetation was not available, occurrence of herbaceous riparian vegetation around all water bodies was assumed, and spray-drift filter potential of this vegetation was applied as shown in Figure 37 (Section 5.3.5.5).

6.4.4.4 Risk Management Scenarios

In Table 24, RM scenarios investigated with the *Xplicit-Aquatic-Model* are summarised. The empirical spray-drift deposition variability (underlying the PDFs derived by Golla *et al.* 2011), the drift filtering by riparian vegetation, effects of drift reduction and buffer zones were assumed independent from each other. Drift reducing technology and buffer zones were applied at field-scale (related to farmer behaviour), and were deterministically defined (no variability), whereas empirical variability of spray-drift filtering of riparian vegetation was assigned to either *Exposure-Path-* (local) or field-scale (Table 23).

Table 24: RM scenarios.

Scenario #	Drift Reduction by Application Technology	Buffer Zone	Spray-drift Filtering by Riparian Vegetation
1	0%	1 m‡	no filtering
2	50%	1 m‡	no filtering
3	0%	5 m	no filtering
4	50%	5 m	no filtering
5	0%	10 m	no filtering
6	0%	1 m‡	low vegetation (EP, F)Δ
7	50%	1 m‡	low vegetation (EP, F)Δ
8	0%	5 m	low vegetation (EP, F)Δ
9	50%	5 m	low vegetation (EP, F)Δ
10	0%	10 m	low vegetation (EP, F)Δ

‡ a naturally present 1 m field-to-WB distance, *i.e.*, no extra buffer zone as RM
Δ Assessed at *Exposure-Path-* and field-scale.

6.4.4.5 MASTEP

MASTEP is an *Individual-Based-Model* (IBM) which was developed in a joint project between the research institute Alterra (WUR 2013), Bayer CropScience (van den Brink *et al.* 2007, Galic 2012) and further sponsors (*e.g.*, Syngenta, P Thorbeck, pers. comm. 2012). MASTEP is a (meta) population model to assess, *e.g.*, recovery of invertebrates after mortality events, induced by a PPP. MASTEP has been configured and parameterised for the waterlouse *Asellus aquaticus*.

"*The model includes processes of mortality, life history, random walk between cells, density dependence of population regulation and, in case of the stream scenario, medium-distance drift of invertebrates due to flow velocity. All parameter estimates currently included were based on expert judgment and the results of a thorough literature review on published information on the ecology of A. aquaticus covering the last 50 years.*" (van den Brink 2011, pers. comm.).

The model is spatiotemporally explicit and accepts corresponding external input. To this end, a MASTEP patch can be 1:1 assigned to an Xplicit receptor (representing a WB segment of 5 m); an output of the eFate module of the *Xplicit-Aquatic-Model* can provide corresponding input.

Technically, MASTEP is implemented in NetLogo (Wilensky 1999). NetLogo runs on the Java virtual machine, as a standalone application or via command line. Preliminary testing has shown that the software can operate as *Associated-Model* with the *Xplicit-Framework* (S Bub, Tier-3 Solutions, pers. comm. 2011). In preliminary testing, the most simple option to run MASTEP was used, that is running as batch-model subsequent to *Xplicit-Aquatic-Model*.

Linking Xplicit to MASTEP was also presented and discussed in the preparation of a postdoc project conducted in the course of the CREAM Marie Curie Initial Training Network ("Mechanistic Effect Models for Ecological Risk Assessment of Chemicals" (CREAM 2013), A Focks, Alterra (WUR 2011) pers. comm. 2011).

6.4.5 Results and Discussion

Results for the exposure part of the study were obtained and are summarised below. Variability of spray-drift filtering of riparian vegetation was assigned to *Exposure-Path*-(local)-scale.

6.4.5.1 Exposure Assessment

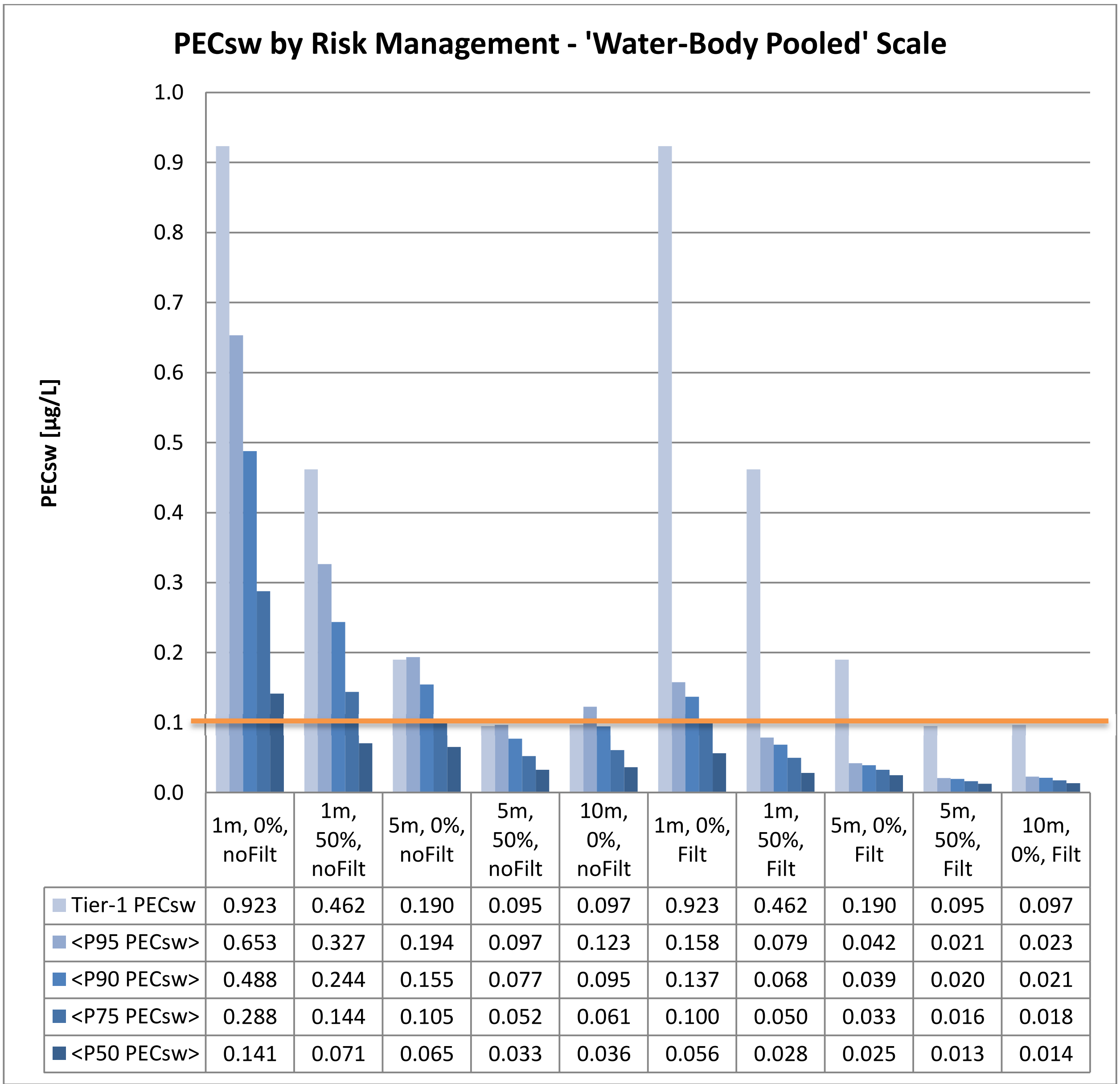
The analysis was conducted at two landscape-scales, (a) the entirety of WB segments as a single set (WB_{pooled} – scale), and (b) by individual WB ($WB_{individual}$ – scale). The $WB_{individual}$ – scale is of particular interest as it can represent an ecologically relevant scale for local hot-spot management (*e.g.*, ranking of water bodies according to their potential risk).

Discussion of risk acceptability predominately focus on the 90th percentile exposure values of a given scale ('P90 PECsw'), as representing a realistic worst-case.

Using the official 'Abdrifteckwerte' (Rautmann *et al.* 2001), which give a spray-drift deposition rate of 2.77% at 1 m distance, and a 0.3 m deep WB, a PECsw_Tier-1 = 0.923 µg/L was obtained, resulting in a TER_Tier-1 = 0.1, which is <1 (requested TER).

WB$_{pooled}$ – scale

Results obtained at WB$_{pooled}$ – scale are summarised in Figure 79, based on the data and methods employed (Section 6.4.4).



	1m, 0%, noFilt	1m, 50%, noFilt	5m, 0%, noFilt	5m, 50%, noFilt	10m, 0%, noFilt	1m, 0%, Filt	1m, 50%, Filt	5m, 0%, Filt	5m, 50%, Filt	10m, 0%, Filt
Tier-1 PECsw	0.923	0.462	0.190	0.095	0.097	0.923	0.462	0.190	0.095	0.097
<P95 PECsw>	0.653	0.327	0.194	0.097	0.123	0.158	0.079	0.042	0.021	0.023
<P90 PECsw>	0.488	0.244	0.155	0.077	0.095	0.137	0.068	0.039	0.020	0.021
<P75 PECsw>	0.288	0.144	0.105	0.052	0.061	0.100	0.050	0.033	0.016	0.018
<P50 PECsw>	0.141	0.071	0.065	0.033	0.036	0.056	0.028	0.025	0.013	0.014

Figure 79: Tier-1 and landscape-scale PECsw in dependence on RM. Landscape-scale PECsw at WB$_{pooled}$ - scale (Px = xth percentile, '<>' represent expectancy values, orange line indicates risk acceptability threshold, a '1 m' buffer indicates the naturally present distance, *i.e.*, no additional buffer as RM; RM scenarios are a combination of buffer zone, application technology and vegetation filtering, *e.g.,* '1 m, 0%, noFilt', Table 24).

Key observations (Figure 79):

- RM alternatives to achieve a TER ≥ 1 (PECsw ≤ 0.1 µg/L):
    - At Tier-1 RA level, 50% drift reduction + 5 m buffer zone, or a 10 m buffer zone.
    - At WB_{pooled} – scale RA level, without filter effect of riparian vegetation, the same RM combinations of drift reducing technology and buffer zones are required as at Tier-1.
    - At WB_{pooled} – scale RA level, the filter effect of riparian vegetation, could lead to lower RM requirements regarding drift reducing technology buffer zone. Either 50% drift reducing technology or 5 m buffer could represent a sufficient protection level.
- WB_{pooled} -scale vs. Tier-1: Without taking into account the RM factors 'buffer', 'technology', 'riparian vegetation', expected P90 PECsw_WB_{pooled} = 0.488 µg/L. This is about half the exposure of Tier-1, and is due to variability of spray-drift depositions, wind directions and local distances >1 m. When imposing buffer zones (5 m, 10 m), this naturally present, 'geometrical' protection converges to the Tier-1 as more local field-to-WB distances tend to occur within these buffer zones. Improving the geodata to better represent small real-world distances is unlikely to affect this results, as in intense arable cultivations ditches often occur in distances of a few metres from fields and are surrounded by fields (Figure 78).
- Effectiveness of RM alternatives:
    - Using a deterministic 50% drift reducing technology simply reduces exposure by 50%. Although the general effect on risk is moderate, it could have a significant mitigation effect on upper percentile spray-drift deposition. This is indicated by the RM alternative 50% reduction + 5 m buffer, for which the P95 PECsw is lower than for the 0% reduction + 10 m buffer option (without RM of riparian vegetation).
    - The effect of buffer zones to reduce spray-drift depositions is substantial (Figure 79) and is documented for the Tier-1 level by Rautmann *et al.* (2001). At WB_{pooled} - scale buffer have an over-proportional reduction effect on high PECsw percentiles. The reason for this 'distance-variability effect' is that the buffer causes a shift in the spray-drift deposition PDFs towards larger distances, which reduces probability density more than, *e.g.*, on average values (Golla *et al.* 2011, Schad & Gao, Section 5.3.5.4). However, the relative reduction effect of buffers, *e.g.*, to the P90 PECsw does not reach the same level as at Tier-1, because the P90 PECsw is already reduced by further factors (wind direction) contribute to deposition reduction. Thus, at landscape-scale RA level, relative reduction due to buffer zones documented by Rautmann *et al.* (2001) cannot be directly applied, *i.e.*, landscape-scale assessments have to be explicitly conducted for the buffer zone in focus.
    - Spray-drift filtering by riparian vegetation can have a large reduction effect on PECsw (Figure 79). On the assumptions on the occurrence and status of riparian vegetation made in this study, 75% of WB segments could be regarded to be protected even without additional RM. When imposing buffer zones based on Tier-1 RA, the landscape-scale analysis of naturally present mitigation factors (*e.g.*, variability of wind direction, distances, riparian vegetation) can quantify protection levels implemented into lower-tier RA scenarios.

At WB_{pooled} – scale, assessing all WB segments as a single set of the regional scale, different scale-dependent variability of spray-drift filtering disappears.

Local, *Exposure-Path* variability can be interpreted as naturally occurring variability, not influenced by human activities. Field-level variability of filtering by riparian vegetation could simulate vegetation maintenance by farmers, changing conditions at his/her field vicinity. Systematic empirical data on the variability of spray-drift filtering and its scale dependencies are proposed to be generated in order to build a sound basis for RM decisions (*e.g.*, maintenance, planting of windbreaks). This could also be of interest for further environmental protection goals, *e.g.,* good water quality in NRW (Section 4.3).

<u>$WB_{individual}$ – scale</u>

Spatiotemporally explicit results obtained at WB segment scale (receptor) are evaluated, reported and discussed at WB scale ($WB_{individual}$ – scale). The WB represents an ecologically meaningful unit for RA and RM. A threshold ('*Individual Threshold*') for risk acceptability of PECsw > 0.1 µg/l (TER < 1) for less than 10% of individual WB length was defined (GeoRISK, Federal Environment Agency, UBA, Schulz *et al.* 2009).

Risk characterisation is given as the probability *Pvio*(PECsw > 0.1 µg/L for >10% of individual WB length) (Figure 80), in dependence on RM ('technology', 'buffer zone', 'filter vegetation'). Probabilities are derived from frequencies obtained from Monte Carlo runs.

Key observations (Figure 80):

- Without RM, about 30% of water bodies occurring in the vicinity of arable fields in NRW have a *Pvio* = 0. About 70% have a *Pvio* > 0, whereof about 30% are of *Pvio* ≈ 1, *i.e.*, for these 30% the criteria will be violated every application season. RM measures 50% drift reduction, 5 m buffer zone or drift filtering vegetation, each as stand-alone, reduce individual risk, yet, do not lead to risk acceptability as a considerable fraction of water bodies still have high *Pvio*. As obtained for the WB_{pooled} – scale, spray-drift filtering by riparian vegetation outperforms alternatives. For the latter, *Pvio* < 0.5 for about 70% of water bodies, *i.e.*, statistically threshold violation occurs every other year.
- When spray-drift filtering by riparian vegetation is present, and either 50% drift reducing technology, or a 5 m buffer is implemented, *Pvio* = 0 for ≈100% of water bodies. This WB individual result supports RM conclusions drawn at WB_{pooled} – scale and emphasis the important role of riparian vegetation for RM, also in view of economic consequences of RM.
- As indicated at WB_{pooled} – scale, imposing a 10 m buffer zone without presence of riparian vegetation leads to P90 PECsw < 0.1 µg/L, *i.e.*, acceptable risk. Still, a few water bodies (<5%) show some *Pvio* ≈ 0.1. However, this is theoretical as it assumes that no other spray-drift reducing factors occur in the real-world, except a 10 m buffer zone (*i.e.*, the water bodies are completely unprotected with water level at ground level).
- The $WB_{individual}$ – scale can clarify questions on aggregation of threshold violations ('Hot-Spot' analysis, Schulz *et al.* 2009). Meeting the assessment criteria at WB_{pooled} – scale is a

necessary precondition to meet the criteria at $WB_{individual}$ – scale (using the same Assessment Endpoints, here, the P90 PECsw), but is not sufficient, as theoretically violations could aggregate in a few water bodies. This can be the case when conditions of water bodies follow a strongly skewed distribution. The geodata enhancement procedure (Section 6.4.7) can contribute to clarify questions on aggregation.

- RM measures can significantly reduce risk of individual water bodies. In the example, risk disappears when a 50% drift reduction or a 5 m buffer zone were imposed in addition to existing filter vegetation. Reversely, having defined risk acceptability criteria, appropriate RM measures can be identified to balance ecological risk with economic cost.

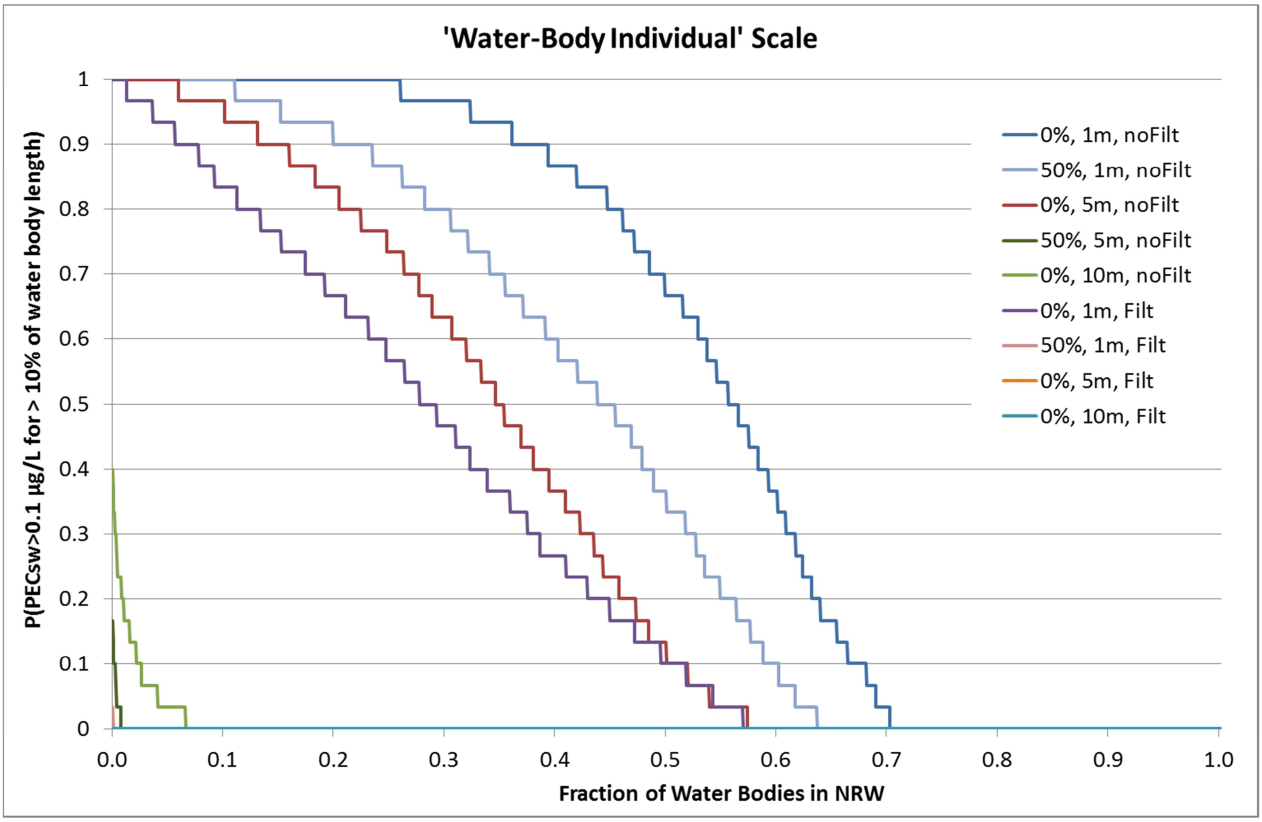


Figure 80: Risk characterisation by individual WB ($WB_{individual}$ – scale) in dependence on RM. Risk given as probability P that PECsw > 0.1 µg/L for >10% of WB length (ordinate), by fraction of water bodies in NRW (cumulated, 1-P). P by RM in order 'technology', 'buffer zone', 'filter vegetation'.

6.4.5.2 Technical Experience

Simulations were conducted at Servers (each: 2 x Intel Xeon CPU E5620, 2.4 GHz, 16 GB memory) using Windows Server 2008 R2 SP1 Operating System. For each *Xplicit-Aquatic-Model* simulation 8 CPU core were available.

Processing time of the *Xplicit-Engine* (comprising 1 *Xplicit-Manager* (*XM*) and 8 Xplicit-Processors (*XPs*), Section 5.3.3.2) was about 9 hours for 30 Monte Carlo runs of a single scenario (whole landscape, specific RM option). Evaluation of raw simulation outcome using *Xplicit-Assess* (*XA*, Section 5.3.3.2) and R (Section 5.3.3.2) took about an hour per assessment. This suggests that, with a total WB length of 192,000 km in the vicinity of arable fields in entire Germany (ATKIS), the system should be capable of processing all water bodies in Germany using an adequate number of CPU core (*e.g.*, 100). There is further potential for optimisation of runtime behaviour, *e.g.*, of workload balancing in the distributed computing module, which is expected to considerably reduce calculation cost.

Approaches built into the LM3 service to improve processing efficiency in Xplicit simulations (Section 5.3.5.2) were used, *e.g.*, to simulate only those *Off-Crop-Receptors* which can receive significant spray-drift deposition (*Off-Crop-Receptors* in *Exposure-Paths*, *Off-Crop-Receptors* in receptor-table, *Off-Crop-Receptors* in total-count-table). In order to reduce processing cost of large landscapes (States, entire Germany), the automation level of the LM3 service needs further improvement.

6.4.6 Conclusions

1. Taking into account limitations regarding thematic and spatial resolution, small-scale topographic geodata (ATKIS) can reveal new insights on aquatic risk which are not available at Tier-1 RA level. The use of the data need to fit to problem formulation. In the present case study, ATKIS data revealed useful to explore the efficiency of different RM alternatives at regional and WB scale. The effectiveness of RM options 'technology', 'buffer zones', and 'vegetation' were preliminary compared. Small-scale geodata can be iteratively improved using high-resolution data and statistically sound sampling procedures, taking scale dependencies into account.
2. At WB_{pooled} – scale, without filter effect of riparian vegetation, the same RM combinations of drift reducing technology and buffer zones are required as at Tier-1. This is likely to hold true even when improving the small-scale geodata, as in intense arable cultivations especially drainage ditches occur in close vicinity to fields. This conclusion depends on the protection level of small manmade drainage ditches and can change in case protection goals of ditches are regarded lower than that of natural streams. When taking filter effect of riparian vegetation into account, RM requirements regarding drift reducing technology and buffer zones are lower than at Tier-1. Either 50% drift reducing technology or 5 m buffer could represent a sufficient protection level.
3. The indicated importance of riparian vegetation as RM for aquatic systems (see also Dutch regulation, Section 4.3.2) is suggested to be further substantiated by systematically generating data on filter effects of (riparian) vegetation in dependence of agricultural and environmental conditions, and by taking scale dependencies into account. This could take

into account eFate processes of substances. Data generation should be guided by the objective to refine landscape-scale modelling, and should be done in relation to geodata improvement. This is an example for an iterative small-scale geodata enhancement (Section 6.4.7). Mechanistic modelling for spray-drift filtering should be considered in future developments.

4 Although the present case study was intentionally kept simple, interacting effects of direction dependent distances, wind variability, spray-drift and drift filter variability emphasised the necessity for local spatiotemporally explicit simulation and for taking scale-dependencies into account, as a basis for refined risk characterisation at higher scales.

5 $WB_{individual}$ – scale addresses an ecologically relevant scale for RA and RM ('Hot-Spots'). The analysis demonstrates the strength of the Xplicit approach in assessing scale-dependent probabilities of quality criteria violations. RM measures leading to risk acceptability at WB_{pooled} – scale reduced the probability *Pvio* that PECsw > 0.1 µg/L for >10% of individual WB length to *Pvio* = 0 for ≈100% of water bodies. Meeting the assessment criteria at WB_{pooled} – scale is a necessary precondition to meet the criteria at $WB_{individual}$ – scale, but is not sufficient, as theoretically violations could aggregate in a few water bodies. This can be the case when conditions of water bodies follow a strongly skewed distribution.

6 RM measures can significantly reduce risk of individual water bodies. In the example, risk disappears when a 50% drift reduction or a 5 m buffer zone were imposed in addition to existing filter vegetation. Reversely, having defined risk acceptability criteria, appropriate RM measures can be identified to balance ecological risk with economic cost.

7 The *Xplicit-Framework* is capable to process large landscapes. Processing all water bodies in Germany (192,000 km in the vicinity of arable fields) should be possible.

8 The present analysis essentially assesses the initial exposure situation due to spray-drift deposition. Future development of refined aquatic risk characterisation can consider eFate and hydrological modelling to take transport and mixing effects into account. Further risk mitigation factors are proposed to be evaluated, *e.g.*, spray-drift 'shielding' effects due to WB geometry (water level is below ground level), variability of wind speed and of spray-drift reduction of application technology. Regionalised cropping statistics ('Agrarsttrukturerhebung ') can allow to assess by individual crop.

9 Preliminary tests suggest to consider spatiotemporally explicit exposure ($PEC_{(r,t)}$) in population modelling for aquatic invertebrates (MASTEP) in order to more realistically represent refuges and areas of high individual-level effects in space and time.

6.4.7 Outlook - Small-scale Geodata Enhancement Cycle

Geodata is a determining factor to the scope of landscape-scale risk characterisation, especially with respect to scale-dependent results and conclusions. Ideally, the spatiotemporal and thematic resolution of data should be adequately fit to scales at which risk characterisation is done: *e.g.*, if RM measures are conducted and administered at units of 100 m WB length, resolution of riparian vegetation data underlying the risk characterisation should be <10^2 m (*e.g.*, HMUELV 2013, 'Gewässerstrukturgütekartierung', Hessian, Germany). Calculations of local potential exposure due to spray-drift typically require resolutions between 10^0-10^1 m (Section 5.3.5.3).

Temporal up-to-datedness of geodata is generally of less concern for the occurrence of general land use/cover types, *e.g.*, arable fields, orchards, meadows or water bodies. For the majority of such entities temporal units of land use change is typically above simulation and RA periods. In case of arable, actual seasonal cropping type (*e.g.*, wheat, rape, etc.) of fields can hardly be kept up-to-date in geodata, nevertheless cropping variability can be sufficiently modelled using cropping statistics and typical crop rotation patterns from agricultural practice. However, temporal variability of the occurrence and conditions of other land use/cover types can be decisive in RA and RM (*e.g.*, maintenance and annual periodicity of riparian vegetation).

A straightforward iterative enhancement cycle is proposed to improve small-scale geodata (Figure 81). Its specific definition should be based on clearly defined objectives.

Preparation steps:

i. Objectives: definition of the goals of the data enhancement based on the purpose of geodata, *e.g.*, "*improved spatial representation of local field-to-WB distance and occurrence of riparian vegetation types, as input for spatiotemporally explicit RA due to spray-drift, as a basis for RM at spatiotemporal scales (100 m, 10 years)*".

ii. Specification: For example, "*mapping of arable field and WB boundaries as well as occurrence of riparian vegetation types at ground resolution ≈10^0 m (≈1:5,000 mapping scale); riparian vegetation as polygons of predefined types (bare, herbaceous, bushes/hedges/trees) using high-resolution remote sensing data (Section 4.5.2.1)*".

iii. Further: Technical details, project management.

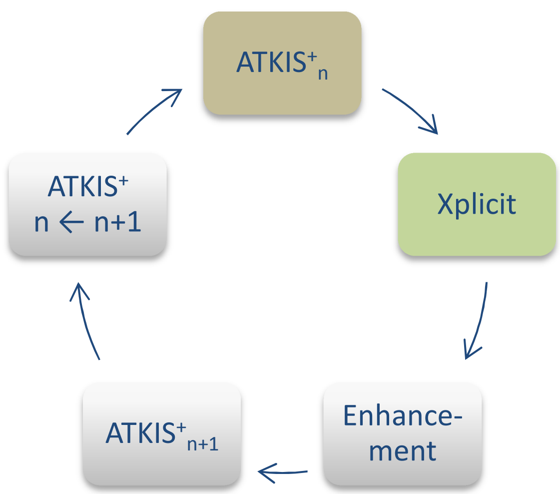


Figure 81: Schematic small-scale geodata enhancement cycle using ATKIS as example. Limitations discovered in an assessment (Xplicit) at status *n* define the objectives of an enhancement which generates status *n+1*, replacing status *n* ($ATKIS^+_{n=0}$ = original).

Geodata enhancement (Figure 81):

i. Definition of objectives and specification.

ii. Random sampling for locations to be enhanced, *e.g.*, using a grid- or segment-based approach. Sampling of grid cells can be purely random, or weighted by metrics derived from the objectives (*e.g.*, co-occurrence index of PPP target areas and habitats indicating potential risk zones).

iii. Selected locations are improved according specifications, *e.g.*, using high-resolution remote sensing data together with manual or (semi-) automated image classification.

iv. Incorporation of improved locations into geodata – alternative approaches:

   a. Direct geometric replacement. Advantage: interactive enhancement of existing data and immediate applicability as input data for Xplicit (via *Landscape-Metric*). Disadvantage: issues with geometric combination of spatial datasets; fractured geodata as a mixture of small- and high-resolution that can result in assessment artefacts; administration of geodata 'branches' as base geodata development is independent from present objectives.

   b. Use of samples as representative empirical model PDFs, representing the variability of the target entities at defined scales (*e.g.*, distribution on the occurrence of riparian vegetation, distribution of local crop-to-WB distances). PDFs can be directly applied in Xplicit taking scale-dependencies into account.

   c. Flexible combination of both: in case entire refined geodata become available for delimited regions (*e.g.*, catchments) procedure (a) can be appropriate, whereas in other regions the representative approach (b) is applied.

In iterative enhancements cycles, the process can stepwise improve risk characterisation, and hence, lead to re-consideration and refinement of RM decisions. For landscape factors like local crop-to-WB distance, or the occurrence of riparian vegetation, *Xplicit-Model* and RM decision endpoints (in defined scales) presumably quickly converge with few iterations. The simple schematic approach can be further shaped using sound statistical sampling methods. The general option to refine the topographic dataset ATKIS has been discussed in joint projects mentioned above (contributors: IVA, UBA, JKI, University Landau, and others, Section 6.4.4.1).

7 Discussion

Ecological risk characterisation in cultivated landscapes built the broader context of this thesis, whereas practical developments were focused on refined risk characterisation in regulatory RA and RM of PPPs (Section 3.1). To this end, in a first section, the current status and developments in general environmental policies and regulations concerning the authorisation and use of PPPs were explored and the landscape-scale was identified as an integrative and operational context-providing unit (Section 4, Section 7.1).

From the regulatory RA and RM schemes (Section 4.3), general requirements for a landscape-scale model approach were derived. On this basis and taking into account the experience gained in recent years in related landscape-scale studies and workgroups (Section 4.4.1.1) as well as with an earlier model version (Schad & Schulz 2011), a landscape-scale modelling framework was developed (*Xplicit-Framework*, Section 5, Section 7.2). This framework is considered to provide the core functionality for spatiotemporally explicit and probabilistic risk characterisation as requested in Section 4.5, from which specific models for specific RA problems can be derived (*Xplicit-Models*, Section 5.4).

The practical work of this thesis concludes with the presentation and discussion of case studies (Section 6) which serve two purposes: (i) to verify the Xplicit concepts and approach from an applied perspective and hence, to show its potential and to identify areas for improvement; and (ii) to present RA problems, results and conclusions as first examples of refined risk characterisation which also relate to potential future scenario development in the context of SPGs (Section 7.3). A brief outlook on possible next development steps in landscape-scale modelling closes the discussion (Section 7.4).

7.1 Demand for a Landscape-scale Risk Characterisation Model Approach

Taking a step back from the current lower-tier regulatory RA schemes of PPPs and putting a focus on forthcoming SPGs together with the multiple perspectives from which environmental and ecological requirements are formulated for services requested from cultivated landscapes ("*food & biodiversity*", Part 1, Section 4.2 and 4.3), the relevance of assessing potential effects of chemical plant protection in their respective context becomes evident.

The more specific required context for RA of PPPs depends on RA goals and problem formulation. It can reach from straightforward local edge-of-the-field scale up to multiple landscape-scales, with multidimensional risk characterisation and taking multiple impacts ('stressors') into account. As an anchor to discussing and defining necessary and sufficient context levels for a problem, the categorical terms *AutContext* and *SynContext* were introduced (Section 4.2): *AutContext* takes the PPP indication specific risk characterisation perspective, from which real-world landscape factors are introduced stepwise which immediately drive risk, whereas *SynContext* takes an ecological entity(ies)-centric perspective (*e.g.*, individual, population, community, biodiversity) which requires characterising all relevant abiotic and biotic factors affecting the entity (*e.g.*, landscape management, cultivation practice, land use, PPP uses, environmental and ecological conditions, dynamics). PPP-specific risk characterisation, RA and RM are then carried out against this *SynContext*. Beyond PPP-specific RA, this view points in the direction of making ecological risk characterisation an explicit component of a RM decision-making process which considers the range of Ecosystem Services of cultivated landscapes.

The *AutContext* perspective relates to the current RA schemes. At the present status of development of risk characterisation, it seems neither sensible nor practical or even possible to strive for the paradigm change in ecological RA for PPPs that might be required by a fundamental transition to the *SynContext*. The related problems are not evaluated in detail herein. For the time being, it seems sensible to start at the *AutContext* perspective and to stepwise introduce real-world conditions (context) in order to refine ecological risk characterisation. This is first of all done with the aim to be consistent with current RA and RM schemes and practices. Example steps are discussed in Section 4.4.2 and are presented within the case studies (Part 3, Section 6). There, the quantification of the large variability of risk begins with introducing landscape factors affecting exposure, while assuming omnipresence of sensitive species and their life stages. The development of future tiered RA approaches and scenarios in relation to SPGs (Reference Scenarios, EFSA 2010a), especially with respect to risk characterisation at (meta-) population, community or even biodiversity levels (*e.g.*, using ecological models), will require further development steps towards *SynContext* (*e.g.*, ModeLink (SETAC Europe Technical Workshop, October 2012 and April 2013), EC 2012b).

The landscape-scale was put into the focus of the conceptual considerations and the operative development as this scale provides the necessary and sufficient context at different complexity levels (Part 1, '*Landscape = Context*', Section 4.2 and 4.4). The term landscape-scale, here, does not refer to a certain metric scale (as, *e.g.*, the local or regional scale); it represents multiple scales occurring in a landscape as well as the multidimensional agricultural, environmental and ecological attributes.

Landscape-scale context can comprise, *e.g.,* land use and management, habitats, cultivation practice (including PPP use), landscape structure, abiotic environmental conditions affecting exposure, eFate and effects, or more complex biotic interactions. Besides providing input data for model process parameterisation, the landscape-scale represents the context into which the model projects its outcome ('*landscape context → model → landscape context*'), thus, immediately relates to RM.

Landscape-scale context introduces new complexity levels to risk characterisation (as required by SPGs). A landscape-scale model has to manage and reduce the complexity along the process of evaluating real-world ecosystems on the one hand, and delivering comprehensible results according to the simple structures of RM decision-making on the other hand. This requires more awareness of risk communication and correspondingly improved skills and tools as the field develops. Risk dimensions in SPGs give a first guidance.

The general requirements for a landscape-scale model for refined risk characterisation focus on the propagation of variability (and uncertainty) of real-world factors affecting exposure and effects on Non-Target-Organisms to variability of risk. Particular attention has to be paid to the role of scales at all assessment levels, from the characterisation of parameter variability to their propagation in the model up to the aggregation of outcome. These considerations led to a spatiotemporally explicit probabilistic model approach, with a core functionality reflecting the recurring structure of RA and RM problems. The specific capabilities of the model should be adaptable to specific RA problems and should enable stepwise introduction of real-world context (complexity). As data availability, process description, the regulatory framework and experience with refined risk characterisation increase, the predictive power of landscape-scale models can develop. An iterative process with milestones seems reasonable in which stakeholders in regulatory RA and RM of PPPs should be involved. With forthcoming SPGs, the work presented in this thesis (including the case studies) and further developments (*e.g.*, ecological modelling), considerations on a milestone regarding necessary context in ecological risk characterisation, RA and RM become self-evident.

7.2 Xplicit Development

The general requirements for a landscape-scale model approach were translated into specific ones which built the basis for a model development ('Xplicit', Part 2, Section 5).

Framework software architecture was chosen to represent the core functionality of spatiotemporally explicit and probabilistic risk characterisation, as required by recurrent RA problem structure. The inherent level of complexity of landscape-scale risk characterisation led to a modular and service-oriented architecture. The variety of regulatory RA and RM problems was covered by using generic *Receptors* as the smallest unit of analysis.

The frequentist approach to probability was realised using a Monte Carlo approach. By taking scale-dependencies in the representation and processing of variability into account, the model enables risk characterisations which comply with the central paradigm of probabilistic approaches, stating that each combination of parameters used as input vector of a trial (simulation run) should represent a case that can occur in the system being modelled ('real-world', Vose 1996). Real-world variability of landscape factors is largely resolved due to spatiotemporally explicit operation, *i.e.*, by numerical discretisation of continuous landscape factors in space and time. A 2nd-order Monte Carlo approach allows for uncertainty analysis.

The *Xplicit-Framework* core is designed to associate external models (*e.g.*, exposure, eFate, effect) in order to derive an *Xplicit-Model*. An *Xplicit-Model* is defined and applicable to a certain RA problem formulation. A *Distributed-Computing* module is part of the *Xplicit-Framework* which allows to run *Xplicit-Models* in parallel on a number of computing units (CPU cores), in order to assure scalability. Analysis of the simulation outcome in different dimensions (*e.g.*, space, time, species, attribute) and at different scales is done in an assessment module ('*Xplicit-Assess*'). Geodata processing (GIS) was designed as a separate service to provide topological input for actual landscape-scale modelling using *Xplicit-Models*. The generic concepts can provide a general basis for harmonisation in refined risk characterisation ("*consistent concepts, multiple application, consistent analysis*").

The developments have created concepts and an approach for landscape-scale risk characterisation ready to be employed in RA and RM problems. For a certain RA purpose, the first steps include the construction of an *Xplicit-Model*, which requires expertise to adapt external models to the *Xplicit-Framework*. The second step represents the application of the *Xplicit-Model*, including parameterisation and input data preparation which essentially results in an *Xplicit-Model-Scenario*. This step requires the same training level as other models used in RA (*e.g.*, FOCUS 2001). Execution of *Xplicit-Model-Scenarios* can be done on a local Personal Computer (PC), using multiple servers in an intranet or on 'Cloud' environments (*e.g.*, Microsoft 2013).

The *Xplicit-Framework* allows to consider defined context (complexity) levels as necessary for a RA. This can start with simple edge-of-the-field scenarios including a few processes and can principally be extended to any appropriate predictive level to characterise ecological risk.

The *Xplicit-Framework* development was accompanied by an excursion into software development methodology (Section 5.2). Agile development methods were found to efficiently structure the development process while keeping the necessary adaptability and flexibility. Together with distinct roles of a software architect, system designer and programmer, this methodological result is recommended for similar scientific model developments.

7.3 Risk Characterisation Using Xplicit

7.3.1 General

The Xplicit concepts and approach were employed for risk characterisation in different problem formulations of regulatory RA and RM. Starting from lower-tier RA levels, the case studies show how risk characterisation can be refined by stepwise introducing landscape-scale context into study definition, processing and risk communication. The case studies also emphasise the necessity to 'plunge into the details of spatiotemporally explicit and probabilistic calculations' to build a sufficiently robust basis for RM at higher organisation levels (*e.g.,* populations).

Lower-tier ('Tier-1') RA levels basically do not allow assessing the extent and likelihood of effects under real-world conditions. This protective assessment level is designed to identify 'true negatives', *i.e.,* PPP uses of low risk. The uncertainty regarding real-world risk is covered by the scenario design. Starting from this level, the case studies significantly increased the knowledge on risk. In a Bayesian view on risk, the case studies led to a new basis of information to the risk assessor with respect to the entirety of data and information available. Therefore, even without having detailed threshold-like decision criteria currently available, the results of the studies provide a supportive part for RM decision-making in uncertain situations.

7.3.2 Non-Target-Arthropods

A case study conducted to refine risk characterisation for Non-Target-Arthropods (NTA) due to the use of a PPP in apple and hops cultivations started at Tier-1 RA level at which unacceptable risk was indicated due to spray-drift exposure (TER < 5, the requested trigger value at Tier-1).

Landscape-scale risk characterisation was conducted on the basis of conservative cultivation regions of high co-occurrence of crop and NTA habitats. At regional scale, the results demonstrated that 3.5% of NTA habitats were expected to be of TER < 5 for hops (6.8% for apple) cultivations. Considering the 90th percentile (P90) as a realistic worst-case exposure value, a TER = 84.6 resulted for the use in hops, and a TER = 10.9 for the use in apple cultivations, which shows that to a large extent NTA habitats are unlikely to receive spray-drift depositions leading to unacceptable risk. At individual habitat (patch) scale, the spatial and temporal recolonisation potential was analysed, which showed that NTA habitat fractions of TER < 5 are to a large extent well connected to habitat fractions of TER ≥ 5 (refuges). Recolonisation can mostly occur from within the same NTA habitat and within about a week. At local habitat segment scale ('receptors'), recurrence frequencies showed that for <1% of receptors, TER < 5 event happens every year, and for <10% of receptors every other year. Risk is apparently of highest variability at local scales. Risk characterisation at this scale supports assessments of potential long-term effects on local populations. Study results consistently show that under real-world conditions, the spatial and temporal extent of TER violation (TER > 5) is limited. Correspondingly, the occurrence of the conditions of the Tier-1 scenario is limited.

The NTA case study provides a first example of how, *e.g.,* the spatial and the temporal extent of risk can be quantified in the context of SPGs (EFSA 2010a, Section 4.3). With their explicitness, the results induce (new) questions on the acceptability of effects in different risk dimensions, scales and with associated probabilities (*e.g.,* would it be acceptable if <10% of habitats show a 1<TER<5 every year?). The use of ecological models in order to explicitly assess population level effects is among the next steps (*e.g.,* ModeLink, SETAC Europe Technical Workshop, October 2012 and April 2013). The study also highlights the necessity for further investigations and research on how to introduce an ecologically reasonable context by other impacts ('stressors') than the PPP in focus (Section 4.4.2). Furthermore, with its large part, in which small-scale geodata were used to transfer results obtained for study regions to the Member State level, the study illustrates methods for scenario development in SPGs context (Reference Scenarios, EFSA 2010a, Section 4.3).

In general, results of such studies can be introduced into generic RM in the context of more general ecological development goals (Section 4.3.3) and can even become an integral part of landscape management considerations (*e.g.,* on the relationship between landscape structure and population vulnerability). Furthermore, predicted risk for NTA due to PPP use can become part of an explicit Ecosystem Service-based RM, *e.g.,* by taking economic risk into account.

7.3.3 Non-Target-Terrestrial Plants

Natural or semi-natural plant communities (Non-Target-Terrestrial Plants, NTTP) occurring in cultivated landscapes meet particular environmental conditions. Depending on cultivation density, plant community habitats are often limited to *e.g.*, herbaceous stripes and patches, hedges, riparian vegetation, groves, or wood margins. Agriculturally managed grassland and meadows represent a further type of plant communities. As part of the cultivated landscape, these plant communities are managed to some extent and are affected by a number of conditions, *e.g.*, habitat sizes, connectivity (isolation), fertiliser, maintenance, mechanical effects, herbicidal effects etc. This encouraged general questions about the driving factors with respect to the management of such plant communities with particular consideration on the role of herbicidal plant protection measures.

A case study was conducted using the Xplicit approach with the goal to take initial steps towards refined NTTP risk characterisation. The case study represents the first step of a project which aims at characterising risk of NTTPs at community level and at introducing more context in NTTP RA and RM. In the case study, variability of ecotoxicological effect data on individual-level and of exposure refines risk characterisation. The second step of the project will propagate individual-level effects obtained in the case study to plant population and community level which are the actual biological entities of RA and RM (EFSA 2010a, 2010b, Section 4.3.2) by means of Individual-Based-Modelling. This already includes aspects of the third step which is proposed to take the view of the ecosystem of plant communities and their agricultural and environmental conditions (*SynContext*, Section 4.2).

Although current Tier-1 RA level for spray-drift already includes a range of species and Assessment Endpoints, it does not allow for risk quantification. Tier-1 is designed to be protective as relative extremes of individual-level ecotoxicological effect and exposure are compared in a TER approach. Visually speaking, the most sensitive Assessment Endpoint of the most sensitive species (covered with an additional Assessment Factor) is located at the edge-of-the-field, downwind, at the point of 90^{th} percentile spray-drift deposition. Obviously, not passing these conditions tells little about real-world risk of plant communities.

The first step of the refined risk characterisation started with the definitions and data at the Tier-1 RA level for spray-drift which was not passed by the test herbicide. An *Xplicit-NTTP-Model* was used to refine risk characterisation by taking into account variability of exposure and individual-level effects (dose-responses of 10 species and 7 attributes). Quantification of effect extent was done for the three risk dimensions *species*, *Assessment Endpoint* (*AE*) and *space*, at edge-of-the-field- and regional-scale. Exposure calculation considered variability of wind directions and of local spray-drift depositions.

At the edge-of-the-field-scale, a small NTTP community of 3 m width occurring downwind from the field was assessed. Only a small fraction of the 70 endpoints (10 *species*, 7 *AEs*) of the plant community showed pronounced effects, among which sublethal were dominating: *e.g.*, at the 90^{th} percentile of the spatial community extent, 2 *species-AEs* showed ≈0.3 effect level (30%), both of which were sublethal; a single survival effect of 0.1<effect<0.2 was observed. At 50^{th} percentile, a single *species-AE* showed effects of 0.2<effect<0.3 (sublethal); survival effects of effect>0.1 were not observed.

At the regional scale, a test landscape of dense arable cultivation was investigated. Only herbaceous NTTP communities were assessed which is conservative as this type frequently occurs in close vicinity to fields and is typically of small spatial extent when compared to, *e.g.*, meadows. Four different NTTP community sizes were assessed, starting at 1 m from field edge, and extending up to maximum distances of 3 m, 10 m, 50 m and 100 m. Parts of the plant communities were found to be at the same risk as at edge-of-the-field-scale. This is obvious, as parts of such plant communities always occur next to the field boundary and receive considerable spray-drift. The influence of variability of conditions at regional-scale is shown *e.g.,* by the 50^{th} percentile effects which are significantly lower than at edge-of-the-field scale. Thus, the regional-scale analysis demonstrates that even for small herbaceous plant communities occurring in immediate vicinity to fields in dense cultivations, natural variability of exposure conditions and landscape structure affects risk characterisation. Regional scale analysis emphasised the importance of habitat size and structure, and hence, of landscape management for plant communities.

The results raised the question as to whether sublethal effects on individual-level, which are limited in *effect magnitude*, *number of species* showing effects, *Assessment Endpoint*, and *spatial extent* can cause unacceptable effects at community level under real-world conditions. An approach was outlined in which the *Xplicit-NTTP-Model* will be linked to an Individual-Based-Model (May *et al.* 2009) in order to propagate the individual-level effects over *species*, *Assessment Endpoint* (*AE*) and *space* to the community level. This is also expected to provide insights for risk characterisation at biodiversity level (EFSA 2010a, 2010b, Section 4.3) and to allow for a broader ecosystem perspective of the plant communities.

The results obtained in the case study demonstrate the added value of landscape-scale risk characterisation to improve understanding of risk in its ecologically relevant dimension under more realistic conditions. As the case study design was developed on the basis of current RA schemes and carries characteristics of the standard (Tier-1) RA level, the results are considered immediately supportive to regulatory RA and RM.

With its potential to assess risk at plant community and biodiversity level taking relevant real-world context into account, the approach can be considered in future scenario development (SPGs, Reference Scenarios, EFSA 2010a, Section 4.3.2). This context can include agricultural, environmental and ecological conditions (*e.g.,* realistic plant communities occurring in cultivated landscapes), as well as structural landscape aspects. Results can also feed the process of defining SPGs for NTTPs (EFSA 2010b).

7.3.4 Non-Target-Aquatic Organisms

Spray-drift depositions represent one of the three main routes of potential exposure of aquatic habitats occurring in the vicinity of fields (FOCUS 2001). As with other habitats of Non-Target-Organisms, the Tier-1 exposure scenario is designed to be protective (Section 7.3.2, 7.3.3). This marks the starting point which is taken up by refined risk characterisation.

The two case studies presented in Sections 6.3 and 6.4 share the common objective of quantifying risk of Non-Target-Aquatic Organisms at ecologically relevant scales. Spatial risk extent is considered to represent risk extent of (meta-) populations, and refers to, *e.g.,* fraction of water bodies for which an Assessment Endpoint is violated. Risk quantification was achieved by introducing real-world data on the co-occurrence of PPP use areas (fields, rails) and water bodies (WBs), and hence, by taking exposure driving landscape factors and their variability into account (*e.g.,* variability of local spray-drift depositions, spray-drift filtering by riparian vegetation, regional wind directions). Variability of spray-drift depositions was represented by empirical models (Section 5.3.5.3) which were based on official data (Rautmann *et al.* 2001).

In the 'Rails' study (Section 6.3), risk for aquatic plants was quantified due to potential spray-drift from the use of a herbicide on the UK rail network. Results of the spatiotemporally explicit analysis were presented at individual WB scale and at a pooled scale, at which WBs were treated as a single set. Different spatial units represented ecological units in the analysis (*e.g.,* all WBs in up to 1 km or 100 m from railways).

The results demonstrate that a TER<1 (indicating unacceptable effects) was obtained for <1% of WB segments of WBs occurring in up to 1 km from railways (<5%, for the 100 m maximum distance). At individual WB scale, the probability of instances of TER<1 to occur at large extent of individual WBs is low for the majority of WBs. This shows that aggregation of effects in individual WBs is infrequent, which is first of all due to the fact that typically WBs only occur with small fractions of their length close to railways (*e.g.*, intersecting rails) and as natural WBs (*e.g.*, streams, ponds) mainly occur at considerable distances. The Xplicit analysis was in agreement with a straightforward spatial analysis on the co-occurrence of railways and WBs.

Results of the spatiotemporally explicit RA significantly improved risk characterisation, and provided a basis directly applicable to RM. This was achieved by characterising risk at the scale of individual WBs, expressed in terms of the probability that a quality criteria is violated (TER<1 for a defined fraction (percentage) of individual WB length). Management options at individual WB scale include, *e.g.*, local adaptation of the herbicide use rate (up to switching-off; using Global Position System, GPS) or generic RM (*e.g.*, adaptation of WB maintenance). The results suggest that the absolute number of vulnerable WB sections is comparably small; hence, RM efforts appear feasible.

Risk characterisation can be provided by WB type. This first assessment has shown that natural streams are generally well protected against spray-drift entries due to the fact that they rarely flow parallel close to railways and due to their riparian vegetation. In contrast, parts of some manmade ditches occur close to rails for some hundreds of meters. This characterisation allows for more explicitness in RM at a broader Ecosystem Services level, *e.g.,* by assessing effects to water plants in man-made ditches (of particular ecological conditions) in relation to the economic value of controlling weeds on railways.

From this study, further research is suggested to clarify which effect levels at which risk dimension are acceptable to conclude a status of 'no unacceptable effects' at (meta-) population level (SPGs, EFSA 2010a). This can be supported by plant (meta-) population modelling as a means to transfer individual level effects measured in ecotoxicological tests to the (meta-) population or even community level.

With respect to the Xplicit approach, the study demonstrates how risk characterisation can be significantly improved compared to the standard Tier-1 RA with manageable effort. This includes the development of an explicit and operative basis for RM. Xplicit can provide a means for corresponding scenario development (SPGs, Reference Scenarios, EFSA 2010a), by which more context can step-wise be introduced (*Aut-/SynContext*, Section 4.2). Landscape-scale risk characterisation studies as presented can also provide a valuable empirical 'knowledge-base' in the process of defining SPGs: *e.g.*, the study provides information on risk of different WB types, indicating that risk of artificial manmade ditches is higher than that of natural streams. Thus, risk of ditches can determine RM measures with potential economic impact. Therefore, and provided that sufficient knowledge on ecological risk and value of WB types is available, differentiation of protection levels might be considered.

A second case study on aquatic risk characterisation (Section 6.4) focuses on assessing RM options. For a test PPP used in arable crops, risk of aquatic organisms was characterised for the entire federal State 'North Rhine-Westphalia' (NRW) in Germany. The study was designed as a pilot study for the use of small-scale geodata (ATKIS) to explore the following main goals: (i) estimation of the distribution of potential exposure due to spray-drift at landscape-scale for a large regional extent (NRW) and comparison to the Tier-1 scenario, as well as (ii) comparison of the efficiency of RM measures. Furthermore, initial steps towards risk characterisation at population level were undertaken by using an Individual-Based-Model (MASTEP, Galic 2012) as effect model in Xplicit.

As RM options, drift reducing application technology (50% reduction), buffer (no-spray) zones (5 m, 10 m), and spray-drift filtering by riparian vegetation were assessed. Effects of technology and buffer zones were implemented deterministically; for drift filtering by vegetation empirical variability was employed (Section 5.3.5.5). WB characteristics were kept as defined in the Tier-1 scenario. Assuming a 10 m buffer (no-spray) zone, the Tier-1 RA level indicated acceptable risk for the test PPP.

Small-scale geodata (ATKIS) can reveal new insights on aquatic risk which are not available at Tier-1 RA level when taking into account their limitations regarding thematic and spatial resolution. ATKIS was shown to be useful to explore the efficiency of different RM alternatives at regional and WB scale. Small-scale geodata can be improved using high-resolution data and sampling procedures, taking scale dependencies into account. An iterative enhancement cycle for small-scale geodata was proposed.

For the entirety of WBs as a single set (WB_{pooled} – scale), without filter effect of riparian vegetation, the same RM combinations of drift reducing technology and buffer zones are required as at Tier-1. This result does not depend on positional accuracy of small-scale geodata because in intense arable cultivations, especially drainage ditches occur in close vicinity to fields. This preliminary RA conclusion depends on the protection level of small manmade drainage ditches and can change in case protection goals of ditches are regarded as lower than that of natural streams. When taking filter effect of riparian vegetation into account, RM requirements are lower than at Tier-1. Either 50% drift reducing technology or a 5 m buffer could represent a sufficient protection level.

The indicated importance of riparian vegetation as RM for aquatic systems (see also Dutch regulation, Section 4.3.2) is suggested to be further substantiated by systematically generating data on filter effects of (riparian) vegetation in dependence of agricultural and environmental conditions, taking scale dependencies into account.

The analysis by individual WB ($WB_{individual}$ – scale) demonstrates the strength of the Xplicit approach in assessing scale-dependent probabilities of quality criteria violations. The individual WB represents an ecologically relevant scale for RA and RM ('Hot-Spots', Schulz *et al.* 2007, 2009). RM measures leading to risk acceptability at WB_{pooled} – scale reduced the probability *Pvio* that PECsw exceeds a trigger of 0.1 µg/L for >10% of individual WB length to *Pvio* = 0 for ≈100% of WBs. Meeting the assessment criteria at WB_{pooled} – scale is a necessary precondition to meet the criteria at $WB_{individual}$ – scale but is not sufficient, as theoretically violations could aggregate in a few WBs. This can be the case when conditions driving exposure of WBs follow a strongly skewed distribution. RM measures can significantly reduce risk of individual WBs. In the example, risk becomes inconsequential when a 50% drift reduction or a 5 m buffer zone are imposed in addition to existing filter vegetation. Having risk acceptability criteria at hand, appropriate RM measures can be identified to balance ecological risk with economic cost.

Although the present case study was intentionally kept simple, interacting effects of direction dependent crop-to-WB distances, wind variability, spray-drift and drift filter variability emphasised the necessity for local spatiotemporally explicit simulation and for taking scale-dependencies into account, as a basis for refined risk characterisation at higher scales.

The *Xplicit-Framework* has proven capable of processing large landscapes. Experience with its scalability should allow to process all WBs in Germany (192,000 km in the vicinity of arable covered in the ATKIS database).

The present analysis essentially assesses the initial exposure situation due to spray-drift deposition taking definitions of the Tier-1 scenario into account. Future development of refined aquatic risk characterisation could consider eFate and hydrological modelling to take transport and mixing effects into account. In addition, further risk mitigation factors are proposed to be evaluated, *e.g.*, spray-drift 'shielding' effects due to WB geometry (water level below ground level), variability of wind speed and of spray-drift reduction by technology. Regionalised cropping statistics can allow for assessing risk by individual crop (*e.g.,* 'Agrarsttrukturerhebung' in Germany) .

7.4 Possible Next Steps

The case studies have illustrated that the *Xplicit-Framework* and *Xplicit-Models* derived from it can make valuable contribution to refine risk characterisation for a range of RA problems. *Xplicit-Models* can be employed for multiple purposes ranging from the definition of scenarios (Reference Scenarios, EFSA 2010a) to processing of such scenarios, up to a higher-tier risk characterisation approach. Furthermore, the spatiotemporally explicit approach can support the future development of the field of ecological RA and RM for PPPs and, hence, serve as a tool to discover and explore related research questions.

Using stepwise methods to introduce more context (complexity) into risk characterisation, the approach allows to take current lower-tier scenario definitions as starting points and to implement risk driving factors. This makes *Xplicit-Models* and *–Scenarios* in current RA problems of PPPs a valuable supportive tool to reduce the overall uncertainty in the RM decision-making process. This higher-tier risk characterisation approach is guided by formal and informal guidance and recommendations of regulatory science (Section 4.3).

Besides the RA problem formulations shown in the case studies, the approach targets on further important fields of refined risk characterisation, *e.g.*, risk to pollinators (bees) or endangered species, as well as biodiversity as an overarching protection goal.

With respect to process description in *Xplicit-Models*, further implementation of well-developed *Associated-Models* is suggested (*e.g.*, eFate, hydrological, ecological models, below). Whether geodata availability is a concern depends on the RA problem formulation. As discussed in Section 4.5.2.1, geodata on land use/cover is generally available at small mapping scale or can be generated in high resolution (large mapping scale) whereas ecological data, *e.g.*, on species occurrence or habitat suitability, need to be improved.

7.4.1 Developments in Regulatory Risk Characterisation

RA and RM of chemical plant protection has come a long way from simple hazard identification to tiered RA schemes (Purdue University 2012). RA schemes in the authorisation of PPPs are basically designed to assess risk due to individual PPP use (Section 4.3). With the introduction of SPGs (EFSA 2010a) which refer to (meta-) population and community level, and with further legislation on environmental protection goals (Section 4.3), the landscape-scale context with its multiple impacts on populations, communities, and biodiversity can become a key RA and RM unit. Therefore, the development of risk characterisation scenarios for individual PPP uses, taking a rather complex ecological and agricultural context into account and at the same time ensuring necessary reduction of complexity towards RM decision-making (Section 4.5.1), is among the major challenges. This requires the cooperation of a number of disciplines (*e.g.*, regulatory, ecology, modelling, ecosystem science, ecotoxicology, etc.). A modular and service-oriented approach, as used in the Xplicit concepts, can support problem structuring and harmonisation of approaches. At some point in the development, a transition to a *SynContext* perspective can become necessary which could require a paradigm change in regulatory RA and RM with a focus on Ecosystem Services (Valerie Forbs, presentation at ModeLink workshop, October 2012, publication in preparation).

More context in ecological risk characterisation, RA and RM does not necessary cause more complex procedures in practice. However, the road leading to operative scenarios and tools addressing more landscape-scale context is likely to require a sufficient level of complexity, with a need for mind-sets of reductionism (ecosystem analyst, theoretical ecology) and holism. First and simple options to consider landscape-scale context have been discussed (Section 4.4.2) and applied in the case studies (Part 3, Section 6).

7.4.2 Research Questions

As shown in Part 1 (Section 4), risk characterisation at landscape-scale is multidisciplinary and comes with an inherent complexity. As a consequence, modularisation defined the overarching principle in concept development and implementation of the Xplicit approach. More context in ecological RA and RM requires efforts ranging from basic and applied research to engineering disciplines. From the experiences obtained in this thesis, the following research fields are suggested:

- <u>Scale-dependent uncertainty propagation:</u> Preliminary results suggest that uncertainty can be partly 'assimilated' in systems of hierarchical scales. Having defined the relevant risk characterisation, RA and RM scales (*e.g.*, regional scale), local parameter uncertainty can be 'trapped' in the scale it occurs; hence, is only partly propagated to relevant RA and RM scale(s). Hypotheses need to be formulated and studied, *e.g.*, on the role of scales, uncertainty distribution characteristics and process non-linearity.
- <u>Scenarios:</u> Risk characterisation scenarios are in direct relation to the purpose of a regulatory RA tier. Landscape-scale approaches (*e.g.*, Xplicit) can support the definition of scenarios at different tiers with different levels of protectiveness and predictiveness. Scenarios will have to be developed with the introduction of SPGs (EFSA 2010a). The required ecological context in future scenarios represents a scientific challenge. The relationship of model (and scenario) purpose and realism needs structured analysis ("*Where are we in the range of protective and predictive risk characterisation?*").
- <u>Model process description:</u> Depending on the model purpose, representation of process details in models associated to the *Xplicit-Framework* (Section 5.3.4.10) can require improvement (*e.g.,* exposure, eFate, populations and community models).

- Data: Data availability is still a crucial determinant of the scope of model application. Generally, any (geo)data improvement supports landscape-scale risk characterisation. However, a structured iterative process is proposed to improve the characterisation of (geo)data requirements from an analysis of forthcoming requirements to landscape-scale risk characterisation, and, conversely, to characterise possibilities for risk characterisation from (geo)data which are available at present or can realistically be generated in the near future. Ecological data, *e.g.,* on species occurrence is of particular concern. Service-orientation in geodata preparation and supply should be considered to improve harmonisation of geodata use in landscape-scale risk characterisation.
- Landscape characterisation: As stated in Part 1 (Section 4), the ecological status of a cultivated landscape is largely driven by its composition, structure and dynamics. With respect to RM, the role of landscape characteristics in PPP risk characterisation should be understood, which also is a prerequisite to scenario definition. The discipline of Landscape Ecology provides approaches to quantitatively characterise landscape structure (McGarigal & Marks 1995) and dynamics.
- Risk communication: Results of landscape-scale modelling, especially when conveyed as maps, are often perceived as the 'truth', although they actually refer to a certain purpose of a (tiered) RA scheme. Aspects of risk perception and new levels of complexity *per se* require new concepts, approaches and skills in risk communication.

7.4.3 (Remote) Future

Developments of further integration of plant protection into future concepts of sustainable agriculture require a corresponding integration of all relevant agricultural activities into ecological RA, and of the ecological risk into broader Ecosystem Service context, *e.g.*, including economic risk.

Systems of higher integration level would allow to explicitly support RM decision-making, *e.g.*, at cost/benefit management level or even higher, taking the range of Ecosystem Services and biodiversity into account (top-down perspective, Figure 82). Such a system could support the 'design' of landscapes according to societal goals as reflected in the Ecosystem Service concept (UNEP 2013), *e.g.*, considering zoning concepts for different weights of balancing economic and ecological goals. At this integration level, the ecological risk characterisation at landscape-scale (Xplicit) itself becomes a service system.

From a bottom-up viewpoint (Figure 82), risk characterisation is developing towards broader landscape-scale context (Section 4.2). This is indicated, *e.g.*, by the introduction of SPGs which emphasise the (meta-) population, community and biodiversity Assessment Endpoints, and hence, inevitably integrate more biotic and abiotic landscape factors affecting populations and communities into risk characterisation. The road could be a stepwise progress in introducing more reality into risk characterisation, defining intermediate milestones as data and models mature.

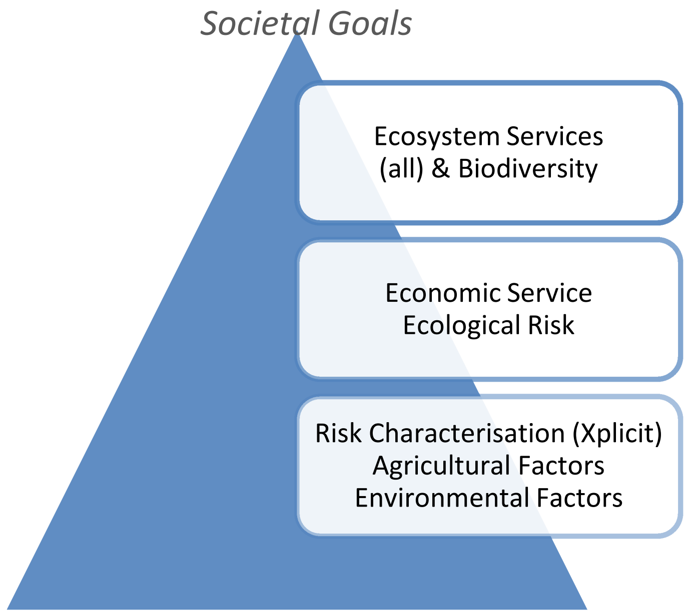


Figure 82: Decision support at different Ecosystem Service integration levels with landscape-scale risk characterisation (Xplicit) as a lower level service.

One possibly close milestone is presented in this thesis, with the development of Xplicit, which operates close to forthcoming SPGs (EFSA 2010a) and which offers the possibility to be employed at different risk characterisation tiers between conservatism and realism, and hence, between protectiveness and predictiveness. This option for stepwise introduction of landscape-scale context into risk characterisation (*AutContext* view, Section 4.2) is illustrated by the case studies.

A more remote milestone could be imagined as a predictive system which is capable to characterise the ecological status in dependence on driving landscape factors (*SynContext* view, Section 4.2), based on sufficient data (services) and model process description (cultivation practice, exposure, eFate, ecological models). At this context level, risk managers could assess individual and generic plant protection strategies in relation to further land management activities and could define appropriate management measures. This level marks the availability of the system as an integrated service in the next level of the 'Ecosystem Service & Biodiversity' guided concept (Figure 82). It could require a paradigm change in regulatory RA and RM by shifting from a PPP-centric assessment (Section 4.4.2) to an 'Ecosystem Service & Biodiversity'-centric one.

8 Conclusions & Outlook

This thesis was initiated with a background of standard (lower-tier) ecological RAs of PPPs which essentially do not allow for risk quantification as they are defined for protective RA purposes. The objectives were found to match to the thinking behind SPGs (EFSA 2010a) which were taken as framing targets for refined risk characterisation.

1 From the regulatory framework affecting the authorisation and use of PPPs, the formula "*landscape=context*" (Part 1, Section 4) was created. From there, the landscape-scale was perceived as a holistic conceptual assessment unit to structure the risk characterisation developments with respect to introduce more context. Three major phases were categorised, an *AutContext*, a *SynContext*, and an 'Ecosystem Services & Biodiversity' phase. The *AutContext* takes the perspective of the PPP indication and aims at stepwise introduction of more realistic conditions. In the *SynContext*, a biological entity (*e.g.*, individual, population, community) is in focus with its relationships to abiotic and biotic landscape factors, of which a PPP use is one of many. An 'Ecosystem Services & Biodiversity' context views the ecological status as one among other services, *e.g.*, economic. At this level, RM can explicitly be done in terms of cost/benefit considerations or taking further Ecosystem Services into account. These categories and related development steps built a suitable basis to define general requirements to a landscape-scale modelling approach.

2 Concepts of modularisation and service-orientation are essential to manage the inherent complexity of a landscape-scale model approach (Part 2, Section 5). An adaptable approach was required to address a range of ecological RA problems. As a software architecture solution, a framework (*Xplicit-Framework*) was created, which provides core functionality for spatiotemporally explicit and probabilistic risk characterisation, together with interfaces to external models and services (*Associated-Models*, *e.g.*, exposure, eFate and effect models, or geodata services). *Associated-Models* are linked to the framework using specific adaptors in order to derive a model which is adapted to a RA problem (*Xplicit-Models*). *Xplicit-Models* are capable of propagating variability (and uncertainty) of real-world agricultural and environmental conditions to exposure and effects using Monte Carlo methods. Hence, they are capable of introducing landscape-scale context to risk characterisation. Scale-dependencies play a key role in landscape-scale processes and were taken into account, *e.g.*, in defining and sampling PDFs. Likewise, evaluation of outcome for risk characterisation is done at ecologically meaningful scales.

3 The potential of the Xplicit approach was demonstrated by case studies (Part 3, Section 6), showing how more realism (context) can be stepwise introduced to refine risk characterisation. The studies mainly operate at *AutContext* level but also including *SynContext* aspects. Starting from lower-tier RA levels, and related to SPGs, the results show how improved *AutContext* can significantly increase risk characterisation for the risk assessor. Thus, the results can provide an evidently supportive part for RM decision-making. For the given RA problem formulations, the results of the studies indicate that exposure and effects are limited in different risk dimensions when taking more realism into account. As a first approximation, the distance to lower-tiers was about one order of magnitude. The studies demonstrate the necessity to '*descend into the details of*

spatiotemporally explicit and probabilistic calculations', in order to build a robust basis for RM decision-making at higher organisation levels (*e.g.,* for populations) and scales. As an overarching principle, scale dependencies need to be taken into account in all aspects, from the characterisation of variability (and uncertainty) up to the evaluation of outcome (actual risk characterisation) and the implementation of RM measures.

4 The adaptability of the Xplicit approach to RA problem formulation, allowing defined levels of complexity, is one of its strengths. The approach can be used as a means for current higher-tier risk characterisation, in the development of scenarios (*e.g.*, Reference Scenarios, EFSA 2010a), or as a future service in a broader 'Ecosystem Service & Biodiversity' context. Results of landscape-scale risk characterisation can be directly applied to RM, *e.g.*, adaptation of PPP use at local scale or generic buffer zones at regional scale. The new levels of complexity require enhanced approaches and skills in risk communication.

5 Future development towards improved realism (in *AutContext* and *SynContext*) first requires improved definition of RA targets (SPGs, EFSA 2010a) and hence, model purposes. It then requires corresponding predictive power of *Xplicit-Models* which defines other needs to be further developed and implemented, *e.g.*, exposure, eFate and ecological processes as well as geodata. Geodata on land use/cover are generally available at small mapping scale or can be generated in high resolution (large mapping scale), whereas ecological data, *e.g.*, on species occurrence or habitat suitability need to be improved. Iterative development processes with clear milestones can provide a methodological means to mutually define the status and realistic development options of geodata and processes on the one hand and the required model predictiveness on the other hand.

6 The propagation of input data uncertainty to model outcome and conclusions is perceived as a major concern (Hart 2001). At landscape-scale, preliminary results suggest that local uncertainty can be 'assimilated' in systems of hierarchical scales. Having defined the operative RA and RM decision scales (*e.g.*, regional scale), local scale parameter uncertainty might be only partly propagated to ecologically relevant scale(s). Research hypotheses need to be formulated and studied, *e.g.*, on the role of scales, uncertainty distribution characteristics and process non-linearity.

9 Acknowledgements

This venture has reached its goal. Saying this, I would like to express my hope that this piece of work marks an intermediate station, a milestone, in the development towards future modelling systems in ecological risk characterisation, assessment and management of PPPs in a broader context of cultivated landscapes, rather than its conclusion.

My journey in landscape-scale modelling started during my time at the UFZ in Leipzig (Helmholtz Centre for Environmental Research, UFZ). There, I had the chance to work and learn in an environment of very competent, dedicated and generous colleagues. The UFZ's Ecological Modelling Department was mainly composed of physicists and biologists, with the fruitful consequence of viewing the same problem from a reductionistic and holistic point of view. These two points of view and their connection have become my personal 'spiritual home' and are, in my opinion important to develop the field of ecological risk characterisation. Many thanks to my colleagues from the UFZ, especially to Roland Brandl, Volker Grimm and Karin Frank for your support for the opportunity to 'travel' between the worlds of nature conservation and computational biology.

The journey continued when I started at Bayer. At that time, I was working on my PhD in ecological modelling (dispersal strategies of plants). The subject was hardly compatible with the requirements of my new job, so I had to put the PhD plans aside. After a phase of 'initial skill adaptation', I realised the potential for development of the scientific foundation and, in engineering, implementation of landscape-scale approaches in different fields of RA and RM of PPPs. I got the chance to contribute to the FOCUS Landscape & Mitigation Group (FOCUS 2007a, 2007b) which provided first recommendations on introducing more realism to RA and RM of PPPs using geodata. On the back of experience obtained from BCS studies, we (BCS and colleagues from industry) initiated a work group at the German Crop Protection Association (IVA), 'GeoPERA', with the aim to examine the potential of georeferenced approaches in regulatory RA and RM. The group closely cooperated with a project of the German regulators, 'GeoRISK' (UBA 2010) which evaluated options on linking PPP-specific RA and RM to generic RM of WBs. Many thanks for the trust that colleagues from industry and authorities have placed in my contribution to these projects. Besides contributing to my first grey hairs, these projects allowed me to learn a lot in the regulatory realm and the constraints on PPP-specific and generic RM.

From these, and further experience gained in BCS projects, I tried to formulate my view on necessary applied scientific and engineering developments for landscape-scale modelling in RA and RM. I got the chance to present my early thoughts at the SETAC GLB conference held at the University Koblenz-Landau (Schad 2006a). Thanks to the organisers of the conference, Prof. Ralf Schulz and Carsten Brühl of the Institute for Environmental Science. The discussions we had initiated our cooperation which led to our first publication on this subject (Schad & Schulz 2011) and, ultimately, to this thesis. Ralf, many thanks for your interest in this subject, our fruitfull discussions and your support in the shaping of my thoughts.

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Understanding the ecological risk of our PPPs beyond the formal requirements of regulatory RA and the contribution to future developments of regulatory RA and RM are among the key goals of the Institute of Environmental Safety (EnSa) at BCS. The EnSa institute supported the development of Xplicit, although the development of a new model approach is not our core business. My sincere thanks go to my superior Gerhard Görlitz and the head of EnSa, Richard Schmuck, for supporting my plans and accepting the uncertainty of succeeding with an innovative project, and for the resources you kindly provided and your trust in my work.

The practical work of the development of what I call today 'Xplicit' started around 2008. Whilst an early version was implemented by me, the current version, with its many different facets, would not have been possible without the contribution of colleagues at BCS and partner institutions. I would like to express my special thanks to the following colleagues:

- Sascha Bub (Institute of Environmental Science at University Koblenz-Landau, Tier-3 Solutions, Tier3 2013) began his contribution at a middle phase of the project. Having successfully programmed parts of the *Xplicit-Assess* component (Section 5.3.3.2) Sascha step-by-step extended his contribution to the implementation and system design of Xplicit. I sincerely want to thank you, Sascha, for your tremendous and dedicated work in implementing Xplicit, your valuable contributions to the software design, and your flexibility in discussing the project in the evenings or on weekends.
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The greatest challenge of this venture was to keep some balance with family life. Despite all interest in the subject, putting the hours into this work against spending them with the family were the bitterest moments. The many hours spent in front of the screen on weekends, in the evenings and on holidays have stretched my family’s understanding and patience. I owe a great debt of gratitude to you, Claudia, for supporting me throughout the process. I was impressed by you, Karl and Theo, on how you managed your disappointment when I couldn't join your plans and on your ways of encouraging me and reflecting about my doing ("*du wirst ja auch mal fertig werden*" (Karl, 8 years), "*meinst du die glauben dir das?*" (Theo, 5 years); after I had explained a certain aspect of this work to him on his request).

Looking back at my personal background, the present work might reflect in a way the down-to-earth environment of my parental home. With all the interest in fundamental scientific questions, typically soon the question concerns me on the applied aspects of a research question (*"Ean woas hot doas fer e Bewandtnis?"*, a question on the purpose of a thing in dialect (Oberhessisch) which has accompanied me through all my life). I am very thankful for having grown up in this environment which also includes a feeling on when a reasonable point has been reached to conclude things ("*Mer muß aach emool ean Sack zoumache*"; one has to know when it's time to 'close a bag').

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11 Appendix

11.1 Requirements Analysis - 'Specification' and 'Quality Attributes'

Table A 1 and Table A 2 provide example higher-level aspects of 'Specifications' and 'Quality Attributes'.

Table A 1: Example aspects of higher-level 'Specifications'.

Subject	Specification
Core functionality	The core functionality of the landscape-scale risk characterisation model should be provided by core software. The core should comprise the program flow logic and control, including that of external modules (models). The core should have a default behaviour which comprises all functionality representing a spatiotemporally explicit and probabilistic landscape-scale model for risk characterisation (see 'Goals' Section 5.3.2.2, and below). The core should include, *e.g.*, model configuration, management of model entities, simulation management including initialisation, time step calculation, data organisation and compilation, distributed computing, and simulation completion. The core model should be extensible for specific model processes (*e.g.*, environmental conditions, cultivation, exposure, eFate, effects) by coding and configuration. In doing so, the model core can become a ready-to-use model for certain RA problem formulations. The core code should be generally considered as not to be altered.
Themes	*Themes* represent key types of activities and processes affecting ecological risk: farmer activity (*e.g.*, PPP use), exposure, eFate, effect. Further *Themes* are given by environmental conditions (*e.g.*, *Weather*). The dependencies of *Themes* should be reflected in their processing sequence: *e.g.*, *Weather* → *Farmer* → *Exposure* → *Efate* → *Effect*. Thus, a predecessor can basically be processed independently from its successor. *Themes* should be represented by modules (below) which should be linked to external process models. These models should be linked to the framework using adaptors. At each time-step the management component should compile the outcome of the different *Themes* (modules) and provide the compiled data as possible input to other modules/*Themes*.
Adaptors	Adaptors should realise interfaces to external models for data exchange and control and should come with two major parts: An internal part should represent the external model to the framework core.
Smallest unit of analysis	The spatial and the temporal domain should be discretised into 'smallest units of analysis' which are subject to model processing. Segments of landscape entities (*e.g.*, fields, habitats) are to be represented by *Receptors* (below). Discrete time steps should represent the temporal discretisation (*e.g.*, units 'day' and 'hour'). Further discrete units for risk characterisation

Subject	Specification
	are to be considered, *e.g.*, biological entities, assessment attributes.
Receptors	Abiotic and biotic *Receptors* are to be distinguished. Spatial segments of habitats of Non-Target-Organisms are referred to as abiotic *Receptors* and should be represented by model entities (objects). An abiotic *Receptor* should provide a sink (and source) of exposure and should have all characteristics that are required to calculate the eFate of substances. This should be done by process models which are linked to abiotic *Receptors*. Abiotic *Receptors* should comprise different compartments (*e.g.*, water and a sediment compartment of a water body). The model core should provide the generic properties and behaviour of abiotic *Receptors* as the basis on which more specific types of receptors can be described (*e.g.*, aquatic or terrestric receptors of different complexity). *Receptors* should be organised by a *Receptor-Management* (below). Biotic *Receptors* should represent Assessment Endpoints (biological entity and attribute, *e.g.*, mortality of individuals) and should be dynamically associated to a certain compartment of one or more abiotic *Receptors* at each time-step. The associated abiotic *Receptors* should provide the biotic *Receptor* with data on substance residues (*e.g.*, concentration, PEC). The biotic *Receptor* should be linked to process models (*e.g.*, TER, RQ, dose-response, mechanistic model) which calculate effects of the defined Assessment Endpoints. The model core should provide the generic properties and behaviour of biotic *Receptors* as the basis to define specific Assessment Endpoints.
Geodata	A geodata module (service) should provide the necessary input data for different process models. This input data should be delivered as required by the process model; *e.g.*, a spray-drift exposure model could require the local distance between a field and a habitat *Receptor* in a given wind direction, together with the intersected land cover types and their widths). Therefore, the geodata module should be extendable to cover the needs for geodata and topological relationships of different process models.
Scales	The model should allow to define discrete spatiotemporal scales (*e.g.*, combinations of 'receptor', 'field', 'region' and 'hour', 'day', 'year') and assign them to model entities, *e.g.*, using a 'Spatiotemporal-Signature'. A 'Spatiotemporal-Signature' type should represent a specific combination of spatial and temporal scale that is assigned to model entities that show scale-dependent behaviour (*e.g.*, PDFs (below)).
PDF	Variability and uncertainty should be represented by a PDF type. This type should allow to define PDFs (and PMFs) and to provide samples taking scale dependencies into account. The use of a 'Spatiotemporal-Signature' type should enable the user to define the spatiotemporal units for which variability (or uncertainty) is represented by a PDF as well as the

Subject	Specification
	spatiotemporal units for which samples can be drawn from this PDF. Standard PDFs should be predefined (*e.g.*, Even, Normal, LogNormal, Gamma, each with truncated derivatives). Also, a random number generator should be provided.
Monte Carlo	Propagation of variability and uncertainty to model outcome should be done using a Monte Carlo (MC) approach. Each MC run should represent an independent sample (MC trial). It should be possible to resolve variability (*i.e.*, drawing samples from a PDF or recalling a previously drawn sample for a given spatiotemporal unit) at some point during runtime; *e.g.*, in case the PPP use by farmers is defined by a deterministic application window within which the actual application date is variable, the decision of the individual farmer should be resolved within the time window (not, *e.g.*, at simulation initialisation). Basically, any model parameter should possibly be representable by a PDF. The outcome of the MC runs should be assessed using an independent assessment component. A 2d-MC approach (nested MC) should be used for uncertainty and sensitivity analysis (UASA).
Configuration	Model configuration should be done using XML (Extensible Markup Language, together with Schema Definitions, XSDs) and using conversion technologies between C#-objects and XML (serialisation/deserialisation). The XML configuration should be prepared using appropriate editors.
Parameterisation	Model parameterisation should be done directly in the configuration or within its building blocks (*i.e.*, 'outsourced' parts of the configuration). Parameterisation should be conducted via custom editor or web-browser user interfaces that are adapted to a specific *Xplicit-Model.*
Weather module	Weather is regarded independent from all other modules. A weather module should provide weather data related to spatiotemporal scales, *i.e.*, it needs to be possible to assign a 'Spatiotemporal-Signature' to reflect weather data variability. Weather data parameters, spatiotemporal resolution and formats (and sources) should be adaptable according to process model requirements.
Farmer module	A 'farmer' entity should represent individual cultivation practices. Basically, farmers' properties should comprise fields they cultivate and cultivation activities should comprise cropping and PPP use. Farmer behaviour should be simulated within a farmer module. The module should be extendable to include further properties (*e.g.*, type of farming) and behaviours (*e.g.*, cultivation activities). The use of PPPs should be characterised close to real-world conditions (*e.g.*, PPPs, crops, uses, technology, etc.). Farmer activities are regarded as independent from the outcome of the exposure, eFate or

Subject	Specification
	effect module, but as being potentially dependent on weather.
Exposure module	Exposure should be calculated source-oriented, with the PPP application as the primary source of exposure. Thus, the 'field' and its discretisation (abiotic *In-field-Receptors*) represent the 'smallest unit of analysis'. This also affects the splitting of the landscape for parallel processing, as the field becomes an undividable unit (for exposure simulation). Applied amounts of active substance(s) in PPP(s) should be allocated to compartments of abiotic *In-field-Receptors* by using corresponding model processes (*e.g.,* amount of sprayed PPP reaching the soil compartment due to interception by plant canopy). Exposure models are to be assigned to *In-field-Receptor* compartments. The *In-field-Receptor* should be used by the exposure module to calculate exposure leaving the field along predefined paths (*Exposure-Paths*, *EPs*). *EPs* represent routes exposure takes starting from an *In-field-Receptor* and affecting one or many *Receptors* which represent habitat segments (*Off-crop-Receptors*). *EPs* should be provided by the geodata service (above). Exposure should be allocated to a compartment of an abiotic *Off-Crop-Receptor* by using a corresponding process model (*e.g.*, instantaneous mixing of active substance amounts reaching a water compartment). Exposure amounts should be represented by corresponding active substance mass and a compartment which 'delivers' this mass (*e.g.*, a water volume in case of run-off). A *Quantity* type should enable to exchange numeric values with assigned units between model entities. The exposure calculation has to take multiple exposure routes (including mitigation) and multiple active substances into account. The exposure module should consider current models used in RA (*e.g.*, FOCUS 2001, Rautmann *et al.* 2001, Großmann 2008). Exposure should be calculated by time-step. The exposure module should accept the output of the farmer module as input and should write its output by *Receptor* and time-step into tables using available data access channels.
EFate module	The eFate of active substances should be calculated for the compartments of the abiotic *Receptors*. Processing should be done by external models. At the beginning, a simple 1st-order dissipation model should be considered. The eFate calculation has to take multiple active substances into account. EFate should be calculated by time-step. The eFate module should accept the output of the exposure module as input and should write its output by *Receptor* (and its attributes) and time-step into tables (*e.g.*, PEC(r,t)) using available data access channels.
Effect module	Effects of Non-Target-Organisms should be calculated for biotic *Receptors*

Subject	Specification
	which should be able to represent effect characterisations of current RA schemes (*e.g.*, TER, RQ, dose-response) and should be prepared to operate forthcoming effect characterisations (*e.g.*, population abundance). Effect calculation should be done by external process models. The effect calculation has to take effects for multiple Assessment Endpoints and multiple active substances into account. Effects should be calculated by time-step. The effect module should accept the output of the eFate module as input and should write its output by biotic *Receptor* and time-step into tables (*e.g.*, effect(r,t)) using available data access channels.
Distributed computing	The landscape should be split into separable portions which are processed in parallel. To this end, the different 'smallest unit of analysis' have to be taken into account (*e.g.,* the 'field' for exposure). Landscape partitioning should be configurable and should be organized by the management component of the software which accesses the geodata module (service). Resulting field lists should be reported in corresponding configuration files (XML) as input for the processing compartments (referred to as 'Processors') and should be stored in a central location which is accessible by the 'Processors'. Besides splitting the landscape, the management compartment should be capable to prepare and publish simulation tasks, to compile the output of the 'Processors' (by time-step) and to terminate a simulation. Further requirements to the management compartment and the 'Processors' should be oriented on Microsoft 'Azure'-like design for parallel computing (Microsoft 2013, *e.g.*, Krishnan 2010, Sirtl 2010, Hay & Prince 2011). Idempotency of the system is required.
Model output post processing	Model output (*e.g.*, PEC(r,t), effect(r,t)) has to be stored at a central location. An independent component should post-process these data for final risk characterisation. Post-processing of individual MC runs should cover data aggregation (*e.g.*, maximum effect by *Receptor* over simulation time), data grouping (*e.g.*, assessment by *Receptor* groups defined in geodata service), and evaluation of distributions (*e.g.*, percentiles of exposure and effect data). Furthermore, distributions of resulting risk endpoints over MC runs should be evaluated (*e.g.*, expectancy values). Evaluation should consider scale dependencies and *Receptor* grouping. The model assessment component should be configured via XML and should operate using external modules (*e.g.*, SQL, R-Statistics, CRAN 2011).

Table A 2: Example aspects of higher-level 'Quality Attributes'

Subject	Quality Attribute
Business rules	The model should fulfil the basic requirements for ecological risk characterisation approaches conducted in the framework of the authorisation of PPPs (Section 4.3 and 4.5.1). These requirements include, *e.g.*, clear and transparent model concepts and architecture with focus on the structure of regulatory RA problems, the consideration of agreed RA procedures (*e.g.,* tiered approach, conservatism, consistency), the capability to use agreed process models (*e.g.,* Rautmann *et al.* 2001), a comprehensible risk communication (*e.g.*, clear and transparent reporting of study results) and the consideration of model verification and validation in context of the model purpose. Approaches should be effective and efficient and should not add more complexity to the RA than necessary. The regulatory environment especially asks for harmonisation of approaches. This should be considered in model concepts by modularisation and service-orientation (*e.g.*, geodata services) in order to establish a basis for agreed modelling endpoints in the multidisciplinary landscape-scale risk characterisation effort. In case simulations are conducted at external platforms (*e.g.*, Microsoft 2013) data security has to be assured.
Ergonomics	Different user groups should be distinguished: (i) The modeller (trained in RA context) who *applies* a predefined '*Xplicit-Model*' (Section 5.4) by parameterisation, and (ii) the '*Xplicit-Model*' builder who derives an applicable model from combining the core model functionality (*Xplicit-Framework*, Section 5.3) with the functionality provided by associated models. Both levels require different expert knowledge and training. Targeting these user groups, configuration and parameterisation of the landscape-scale model should be clear and unequivocal. Parameterisation should be supported by a user interface (*e.g.*, editor, web-browser). Pre-prepared template configurations should be provided to support simulation preparation and post-processing of outcome for ultimate risk characterisation. The translation of a RA problem formulation into an adapted landscape-scale modelling approach should be possible with manageable effort and training. During runtime and after successful completion, the system should provide feedback to the user (*e.g.*, info on processed steps, progress bar, etc.). Model runtime cost should be minimised, *e.g.*, by parallel processing, efficient use of memory and storage, and clearing-up after simulation completion.
Infrastructure	The model should be potentially executable on all Operating Systems that provide a Microsoft .NET Framework environment (Microsoft 2012b). This applies to common Microsoft Operating Systems (*e.g.*, Windows 7, Server 2008) and further systems, *e.g.*, Xamarin 2012. The model should be executable at 32-/64-bit Personal Computers (PCs), servers or cloud platforms (*e.g.*, Microsoft 2013) and should allow even large

Subject	Quality Attribute
	amounts of data (e.g. due to the simulation of large and detailed landscapes) to be processed. Preparation of configuration (XML) and parameterisation files should be done with (XML) editors or a web-based user interface. Modelling data should be stored file-based or in a central database (*e.g.*, RDBMS, Oracle, Microsoft SQL Server, Microsoft SQL Azure). Running the model should be possible with common network bandwidth. As the model simulations are basically reproducible (within the propagated variability), exceptional requirements to system failure do not apply. Data and operation security is likewise to other models used in regulatory RA (*e.g.*, FOCUS 2001).
Modularity & Service-orientation	The multiple disciplines involved in a landscape-scale risk characterisation and the inherent complexity levels as well as the requirements of harmonisation (above) should be addressed by system modularity. Independent modules should conceptually be considered as stand-alone services. Modular concepts should be reflected at any system design level, starting from the separation of the entire model approach into independent components, over functional modules operating different *Themes* (Table A 1, above), down to classes (Object-Oriented-Programming). Real-world objects of the ecological RA domain should be reflected in corresponding model objects (*e.g.*, field, PPP, farmer, habitat segment).
Scalability	The model should be capable to process different landscape (data) extents ranging from, *e.g.*, local (edge-of-the-field) scenarios, to cultivation regions ($\approx 10^2$ km^2), up to multiple cultivation regions or data at Member State extent. The model should be capable to operate 10^6 *Receptors* with moderate resources (*e.g.*, up-to-date multiple core Personal Computer) and 10^7 *Receptors* with extended resources (*e.g.*, >10 CPU cores, >10 GB memory for the management and assessment component).
Data	The typically large data amounts coming with landscape-scale modelling (*e.g.*, $\approx 10^0$-10^2 GB) should be managed by cost effective means while maintaining data accessibility and integrity. Data storage during a RA project lifespan (*e.g.*, configuration, parameterisation, model version, raw and processed outcome) and data archiving (*e.g.*, selected data of direct relation to RA and RM decision) should be considered.
Maintenance	Assuring good maintenance should consider three maintenance categories: *corrective* (reactive due to problems), *adaptive* (to keep the software usable in a changing environment) and *perfective* (*e.g.*, to improve performance) (E.B. Swanson in Wikipedia.org). This should be achieved by clear software architecture and system design including modularity and service-orientation (above), Object-Oriented-Programming, an intelligible coding style and an appropriate documentation.

11.2 Overview on *Associated-Models and -Services*

Table A 3 provides a brief overview on the currently available functionality of modules and *Associated-Models* and *–Services*.

Table A 3: Overview on currently implemented module functionality with respect to the properties and behaviour of major landscape-scale model entities.

***Theme*/Entity**	**Module Objective, Functionality, *Associated-Model/–Service* Characteristics**
Receptor (abiotic)	Module objective: Characterisation of properties and behaviour of abiotic *Receptors*. *In-field-Receptors* (representing field segments): • Air compartment as active substance mass repository for exposure due to spray-drift; soil compartment, as active substance mass repository for exposure due to run-off; • dissipation eFate model; • allocation model to assign active substance mass to compartments after PPP application event. *Off-Crop-Receptors* (representing Non-Target-Organism's habitat segments): • Simple aquatic *Receptor* (static water body segment with instantaneous dilution of active substance after exposure entry event, dissipation eFate model); • simple terrestric *Receptor* (Non-Target-Arthropods (NTA), Non-Target-Terrestrial Plants (NTTP), Vegetation-Dilution-Factor (VDF), dissipation eFate model).
Weather	Module objective: Provide weather data to other *Themes*. Current models and services are based on data records (tabular data from, *e.g.*, FOCUS (2001), DWD (Deutscher Wetterdienst), MARS project (JRC 2012) or PDFs.
Farmer	Module objective: Characterisation of farm management properties and behaviour (*e.g.*, cultivation practice). Farm size model: Different types of field-to-farmer association comprising 1:1 and n:1 (number of fields-to-farmers), with random and or predefined deterministic association (external geodata) and consideration of field types. Crop-rotation model: Crop-rotation schemes can be configured taking land use statistics at regional scale into account (external geodata). Plant protection measures (PPM) model: Each farmer builds its personal PPM calendar (Section 5.3.4.11).
Exposure	Module objective: Representation of exposure processes causing active substance entries into habitats of Non-Target-Organisms (*Off-Crop-Receptors*).

<table>
<tr><th>Theme/Entity</th><th>Module Objective, Functionality, Associated-Model/–Service Characteristics</th></tr>
<tr><td></td><td>Spray-drift exposure models:
Simple deterministic 'Rautmann 90th Percentile Deposition' (power function model, Rautmann et al. 2001, JKI 2013).
'Schad & Gao' probabilistic model (Section 5.3.5.4).
'JKI' probabilistic model (Golla et al. 2011).
'Spray-drift filtering' models (Section 5.3.5.5).
Run-off exposure models:
'FOCUS-Type' (Focus 2007a, 2007b).
'EXPOSIT-Type' (Großmann 2008).</td></tr>
<tr><td>EFate</td><td>Module objective: Characterisation of eFate processes of active substance in Receptor compartments.
Simple substance dissipation model (1st order; DT50 [days]).
Simple water phase instantaneous substance dilution model.</td></tr>
<tr><td>Effect (biotic Receptor)</td><td>Module objective: Representation of Assessment Endpoints.
Effect models are referenced by biotic Receptors which represent ecological Assessment Endpoints (Section 5.3.4.9).
TER, RQ calculation (Toxicity Exposure Ratio, Risk Quotient; ECx).
Dose-response models (e.g., Log-Logistic).</td></tr>
<tr><td>Risk Characterisation</td><td>Module objective: Evaluation of spatiotemporally explicit outcome of Xplicit-Model simulations using Xplicit-Assess (XA, Section 5.3.4.4).
Data aggregation (e.g., minimum, maximum, percentiles, Time-Weighted-Averages, etc.) in different dimensions (e.g., space, time, Assessment Endpoints).
Data upload to data services (e.g., RDBMS, files).
Data combination (e.g., SQL statements against Landscape-Metric data, Section 5.3.5.2).
Statistical evaluations and visualisation using R-Modules (e.g., expectancy values, confidence bounds; CRAN 2011).
Geo-processing to assess potential recolonisation distance, Xplicit-Distance (Section 5.3.5.6).</td></tr>
<tr><td>Geodata</td><td>Geodata service to provide land use/cover data, their discretisation and topological relationship for Xplicit-Model parameterisation.
Landscape-Metric Service (Section 5.3.5.2).</td></tr>
</table>

11.3 Spray-drift Model (Schad & Gao)

11.3.1 Characterisation of *A Priori* groups

Table A 4: Characterisation of *a priori* groups regarding trial conditions 'Wind-speed', 'Pressure', 'Technology'

Crop	Group	Pressure	Wind-speed	Technology
Arable	1-1-1	moderate	moderate	1
Arable	1-1-2	moderate	moderate	2
Arable	1-1-4	moderate	moderate	4
Arable	1-2-1	moderate	high	1
Arable	1-2-2	moderate	high	2
Arable	2-2-2	high	high	2
Arable	2-2-3	high	high	3
Hops	1-2-1	moderate	high	1
Hops	1-3-1	moderate	very high	1
Hops	2-1-2	high	moderate	2
Hops	2-2-2	high	high	2
Orchards-late	1-1-2	moderate	moderate	2
Orchards-late	1-1-3	moderate	moderate	3
Orchards-late	1-2-1	moderate	high	1
Orchards-late	1-2-2	moderate	high	2
Orchards-late	2-1-2	high	moderate	2
Orchards-late	2-1-4	high	moderate	4
Orchards-late	2-2-2	high	high	2
Orchards-early	1-2-1	moderate	high	1
Orchards-early	2-1-1	high	moderate	1
Orchards-early	2-2-1	high	high	1
Orchards-early	2-3-1	high	very high	1
Vines	1-1-2	moderate	moderate	2
Vines	1-2-1	moderate	high	1
Vines	1-2-2	moderate	high	2

11.3.2 Statistics and Graphs for Lumped Analysis

Arable

Table A 5: PDF parameters and statistics, 'Lumped-analysis' - arable

	1 m	3 m	5 m	7.5 m	10 m	15 m	20 m	30 m	50 m	75 m	100 m
normal											
mean	1.208	0.424	0.296	0.182	0.145	0.060	0.067	0.045	0.037	0.015	0.014
sd	1.084	0.307	0.218	0.137	0.110	0.055	0.061	0.043	0.033	0.012	0.009
p	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000	0.000	0.000	0.000
D	0.168	0.138	0.134	0.149	0.133	0.196	0.147	0.154	0.134	0.163	0.173
BIC	1062	1062	179.2	-93.22	-385.7	-788.2	-256.2	-1399	-1761	-1668	-938.9
lognorm											
mean	-0.136	-1.104	-1.475	-1.961	-2.239	-3.193	-3.132	-3.590	-3.785	-4.479	-4.479
sd	0.805	0.717	0.741	0.750	0.847	0.920	1.006	1.098	1.127	0.758	0.607
p	0.014	0.371	0.690	0.883	0.209	0.082	0.008	0.000	0.002	0.886	0.680
D	0.084	0.049	0.032	0.031	0.047	0.133	0.074	0.097	0.090	0.046	0.057
BIC	758.4	-0.962	-350.3	-569.3	-993.0	-325.4	-1729	-2107	-1875	-1058	-1129
gamma											
shape	1.686	2.185	2.081	2.100	1.762	1.492	1.293	1.167	1.165	1.946	2.248
rate	1.395	5.153	7.022	11.55	12.13	25.08	19.20	26.01	31.54	129.8	164.2
p	0.000	0.053	0.253	0.217	0.170	0.309	0.088	0.016	0.357	0.188	0.184
D	0.128	0.072	0.045	0.056	0.049	0.102	0.055	0.069	0.045	0.086	0.086
BIC	794.9	11.29	-338.3	-572.8	-1018	-326.8	-1739	-2141	-1925	-1049	-1112
beta											
alpha	1.659	2.154	1.837	2.038	1.737	1.150	1.251	1.130	1.233	1.558	2.353
beta	135.3	504.5	618.0	1110	1189	1932	1827	2475	3439	9639	16516
p	0.000	0.051	0.286	0.161	0.191	0.026	0.111	0.025	0.211	0.127	0.041
D	0.129	0.072	0.044	0.060	0.048	0.155	0.053	0.065	0.052	0.093	0.110
BIC	796.5	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

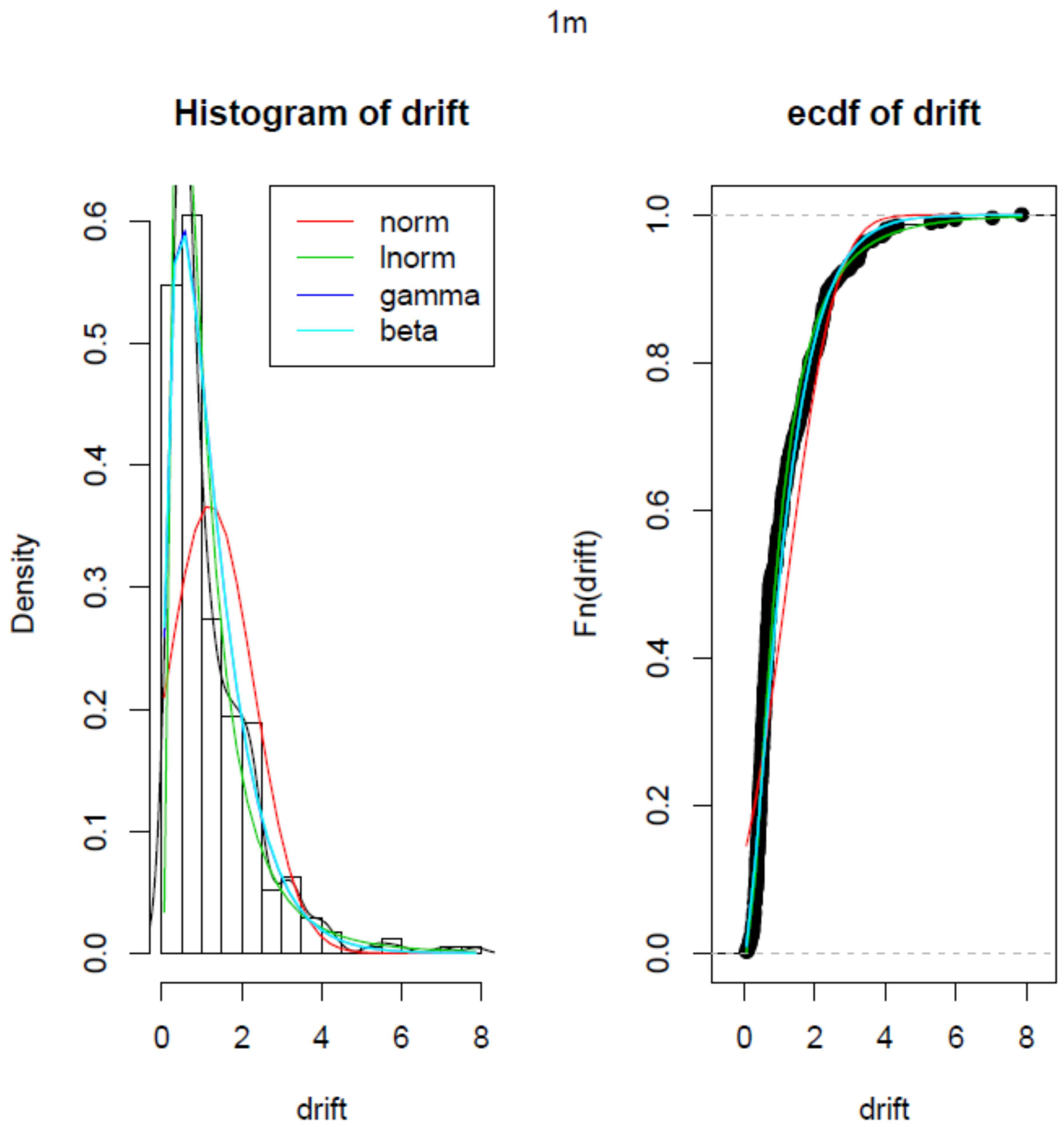


Figure A 1: Illustration of fitted distributions for arable at 1 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

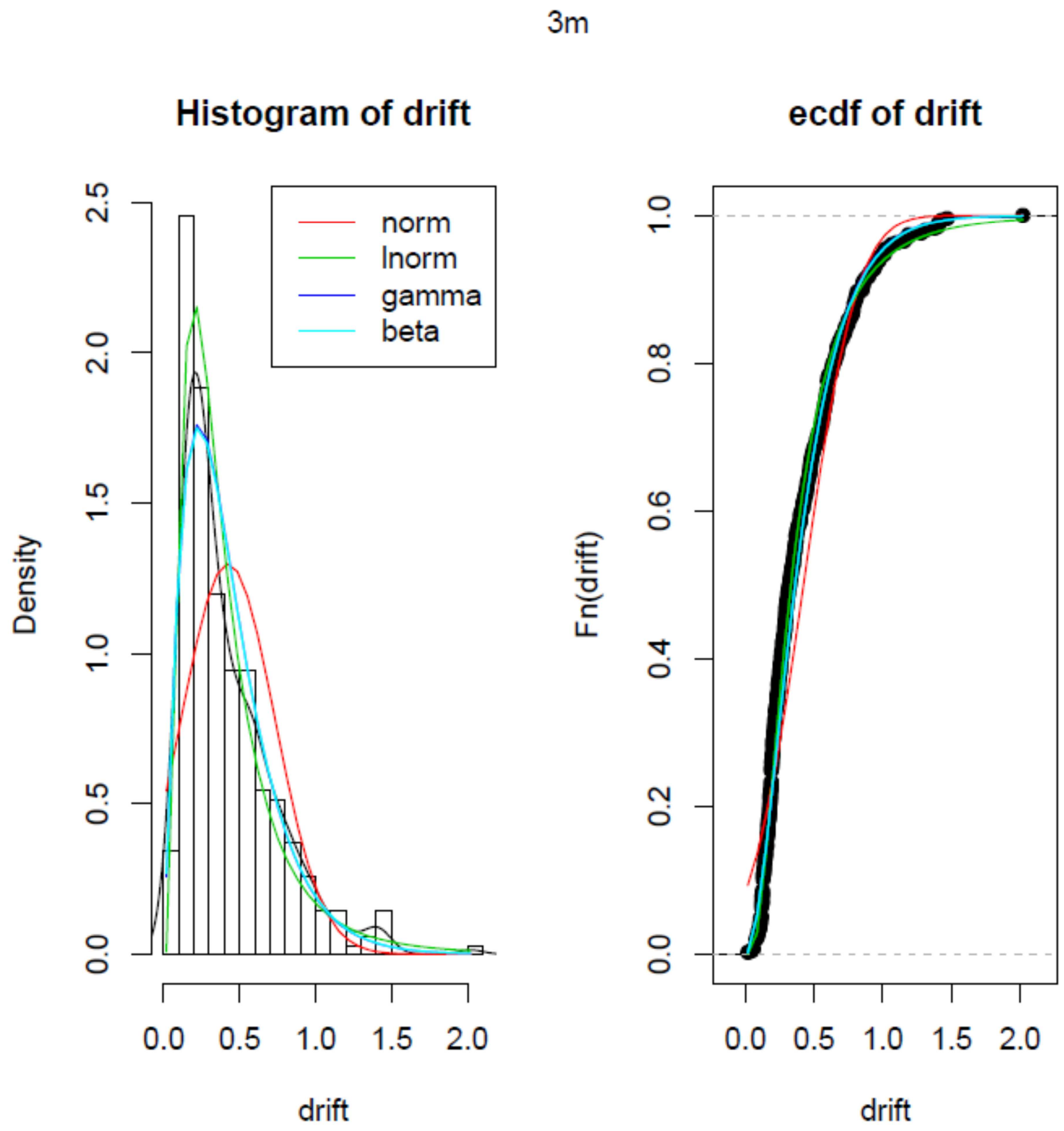


Figure A 2: Illustration of fitted distributions for arable at 3 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

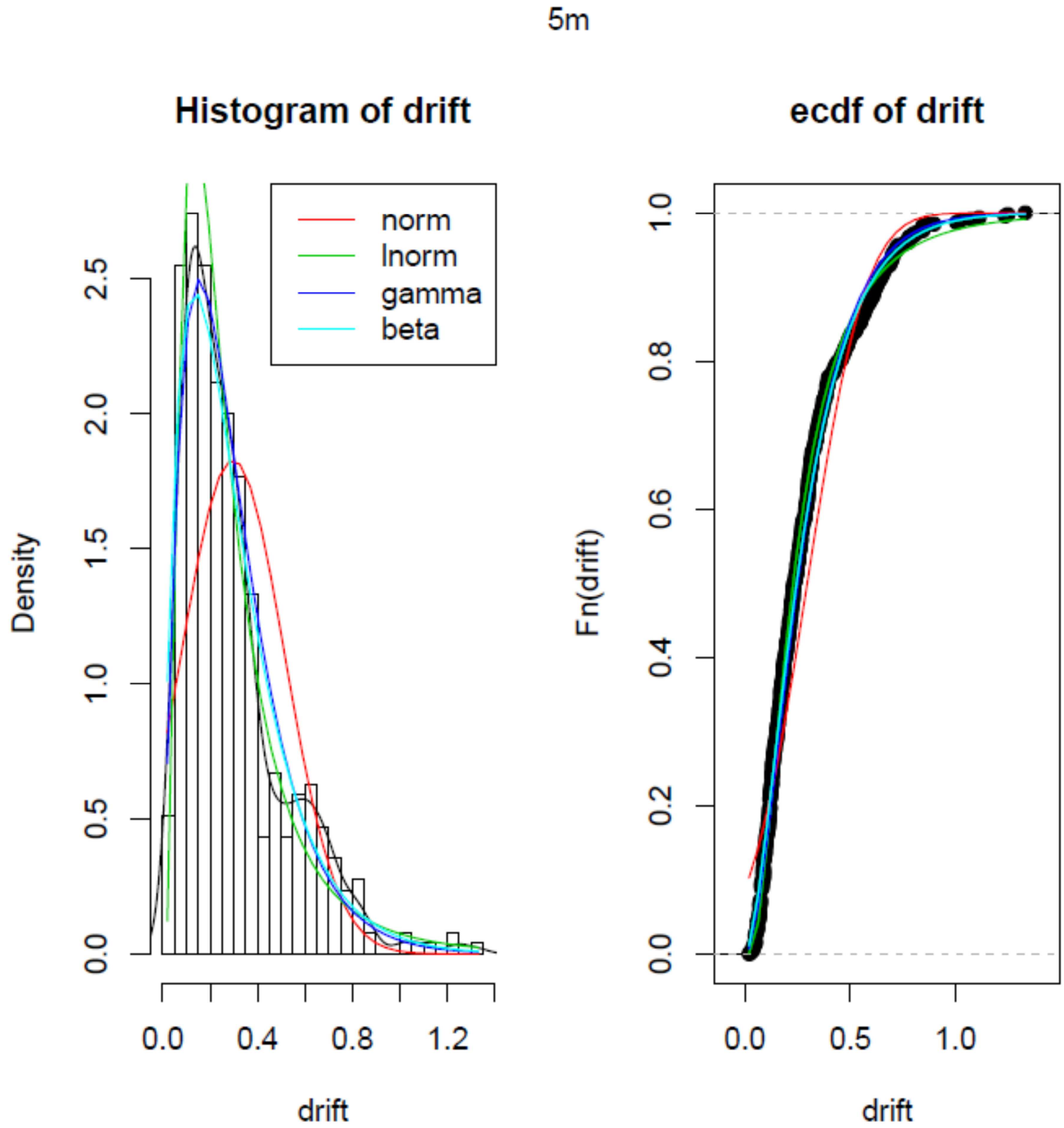


Figure A 3: Illustration of fitted distributions for arable at 5 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

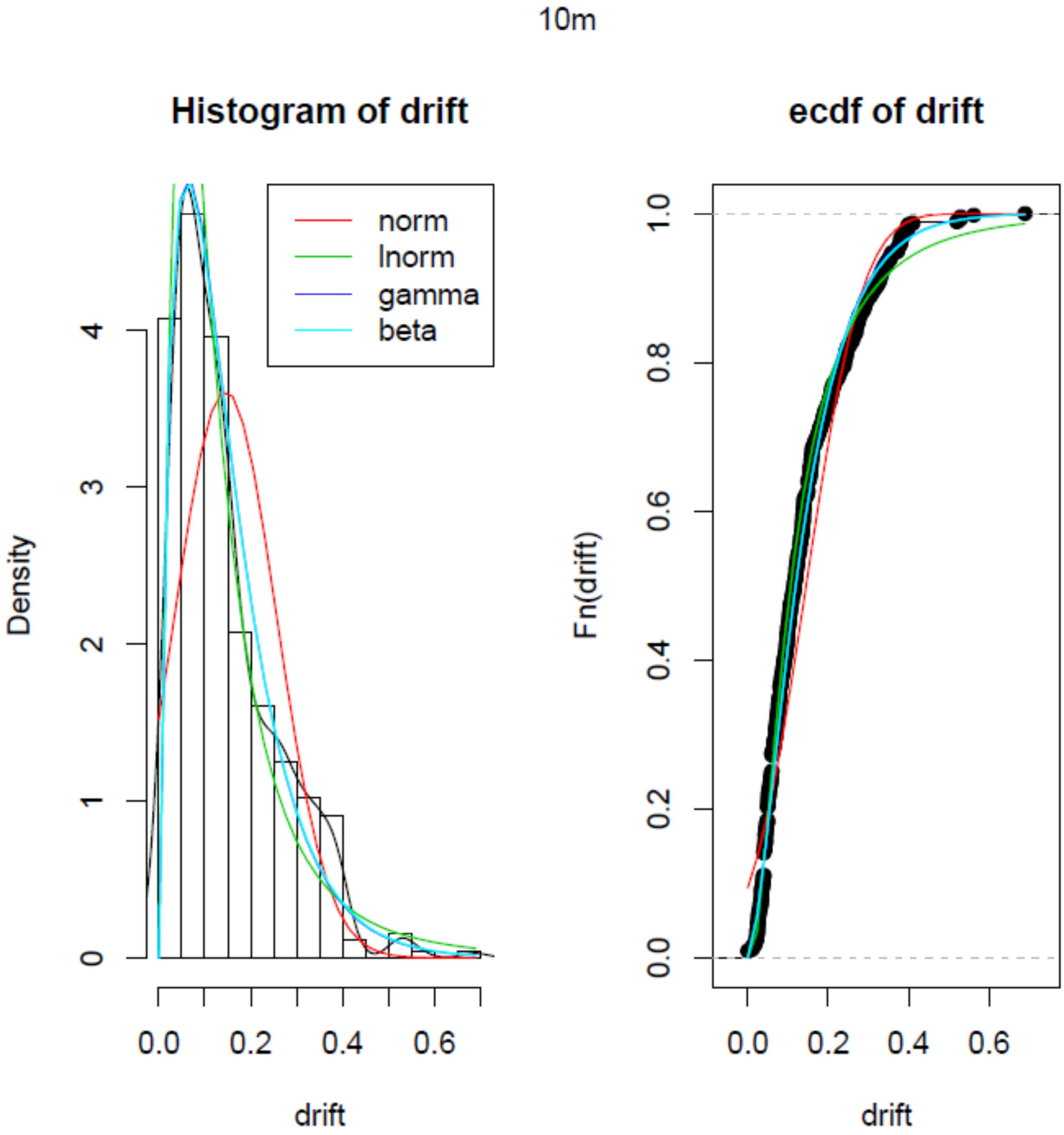


Figure A 4: Illustration of fitted distributions for arable at 10 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

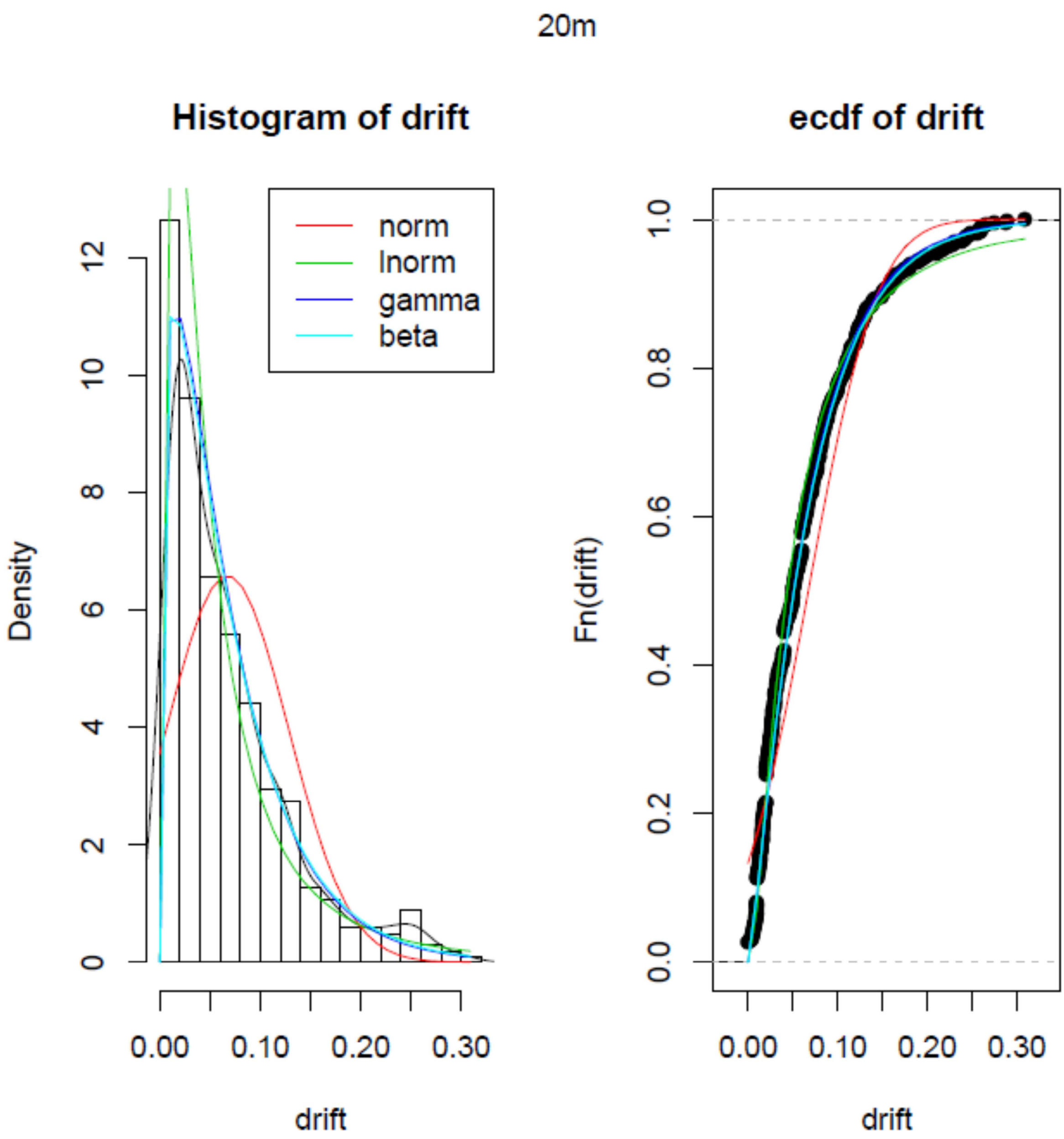


Figure A 5: Illustration of fitted distributions for arable at 20 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

Hops

Table A 6: PDF parameters and statistics, 'Lumped-analysis' – hops

	3 m	5 m	7.5 m	10 m	15 m	20 m	30 m	50 m
normal								
mean	11.630	7.638	4.632	3.268	1.647	0.917	0.340	0.078
sd	6.439	3.654	2.539	1.913	1.236	0.866	0.456	0.082
p	0.131	0.042	0.027	0.207	0.016	0.002	0.000	0.000
D	0.121	0.144	0.152	0.105	0.161	0.183	0.267	0.207
BIC	619.39	514.02	446.28	435.19	312.47	271.93	126.77	-212.50
lognorm								
mean	2.321	1.930	1.379	1.003	0.175	-0.528	-1.657	-3.000
sd	0.509	0.453	0.587	0.645	0.889	1.012	1.079	0.984
p	0.780	0.938	0.229	0.244	0.082	0.323	0.623	0.088
D	0.068	0.055	0.108	0.101	0.131	0.094	0.078	0.123
BIC	578.94	484.91	430.35	417.95	283.65	195.19	-21.227	-319.79
gamma								
shape	3.919	5.021	3.411	2.923	1.689	1.273	0.997	1.266
rate	0.337	0.657	0.736	0.894	1.026	1.389	2.933	16.316
p	0.494	0.495	0.541	0.728	0.630	0.764	0.088	0.304
D	0.086	0.086	0.083	0.068	0.078	0.066	0.130	0.096
BIC	585.48	488.11	424.44	409.45	274.67	193.89	-5.535	-314.59
beta								
alpha	3.388	4.595	3.255	2.830	1.671	1.262	0.552	0.885
beta	25.61	55.47	66.99	83.75	99.91	136.37	161.74	1138.9
p	0.439	0.412	0.488	0.700	0.652	0.743	0.004	0.051
D	0.090	0.092	0.087	0.070	0.076	0.067	0.182	0.134
BIC	588.38	489.43	424.61	409.49	274.61	194.02	NA	NA

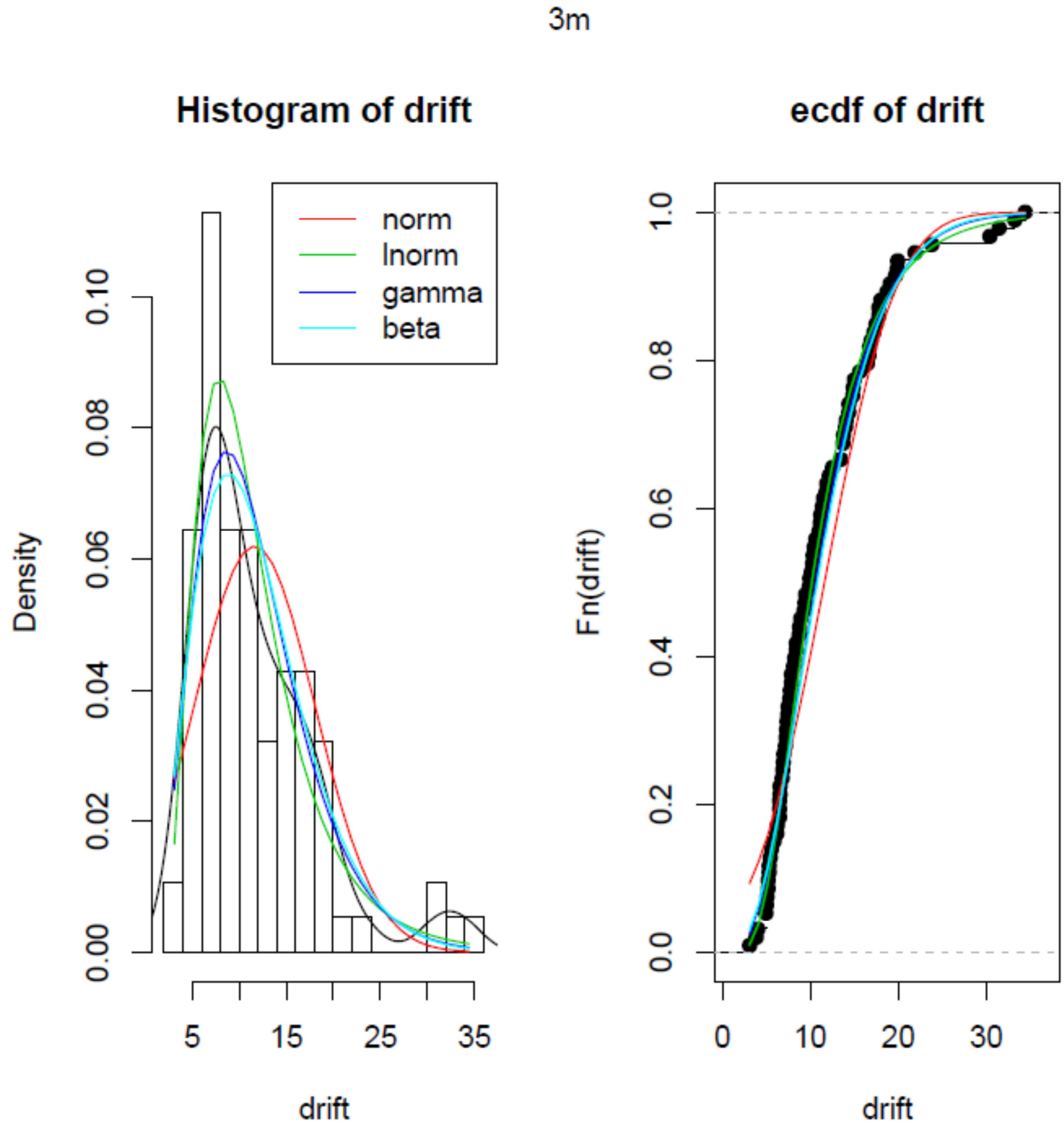


Figure A 6: Illustration of fitted distributions for hops at 3 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

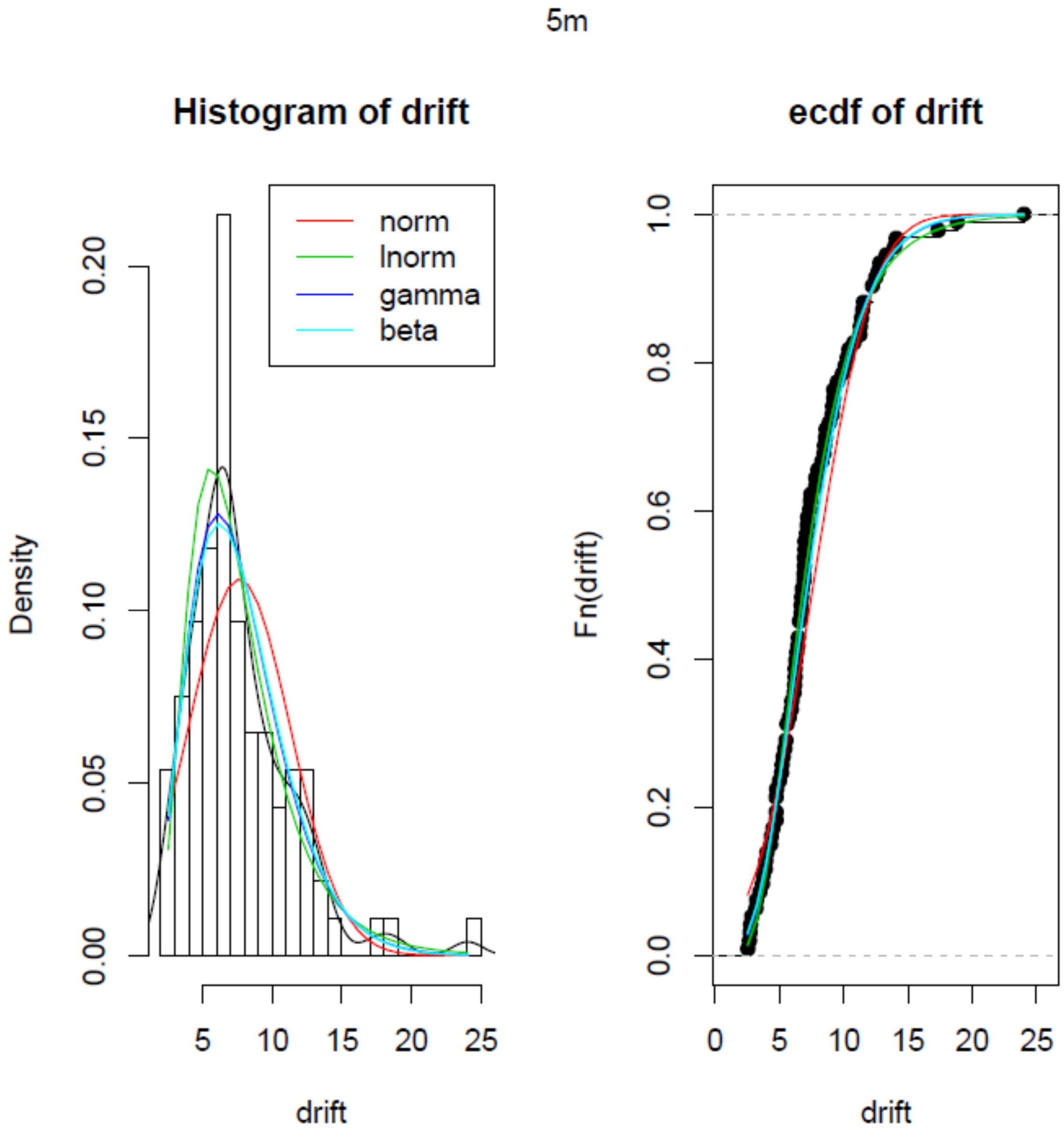


Figure A 7: Illustration of fitted distributions for hops at 5 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

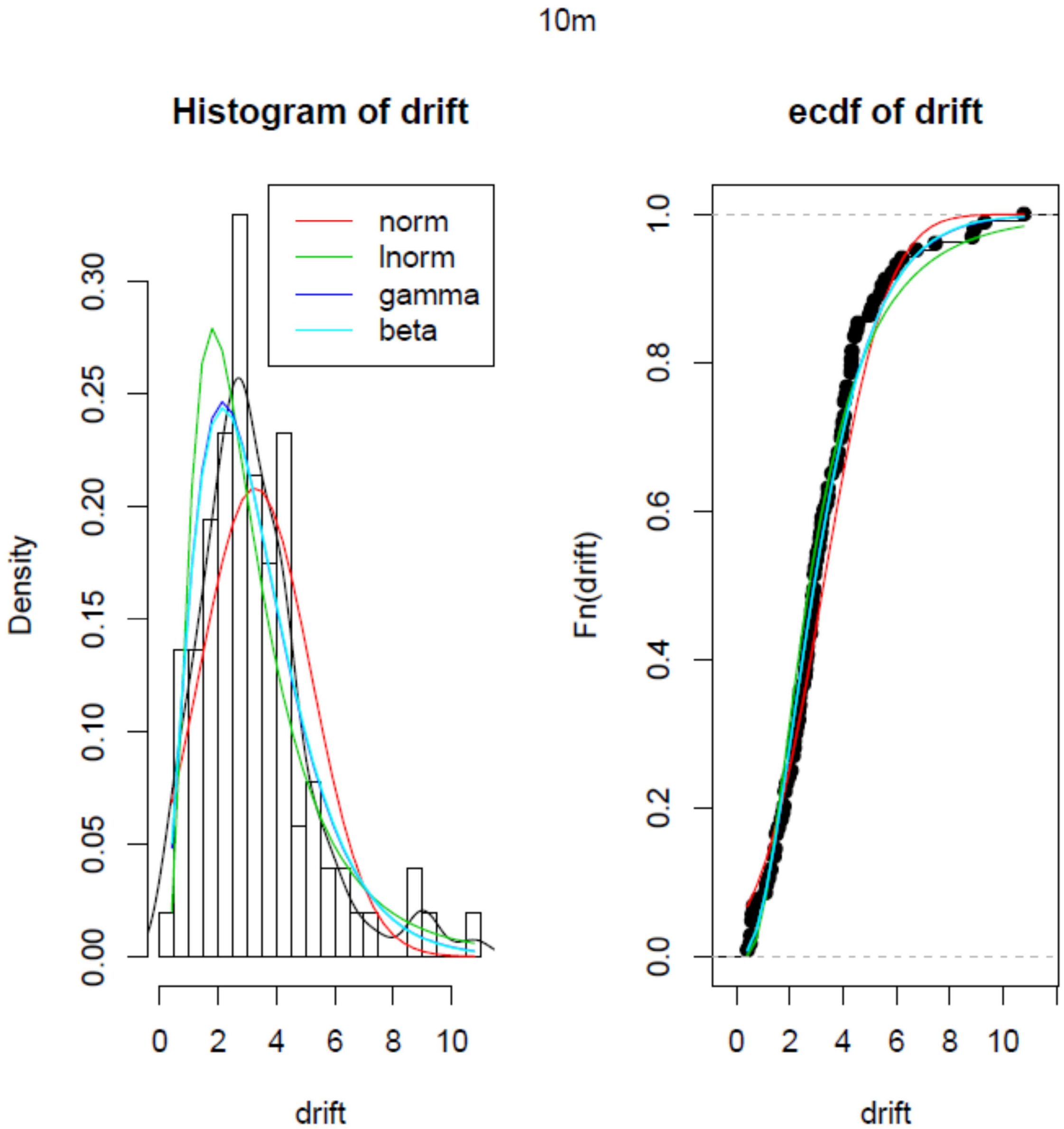


Figure A 8: Illustration of fitted distributions for hops at 10 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

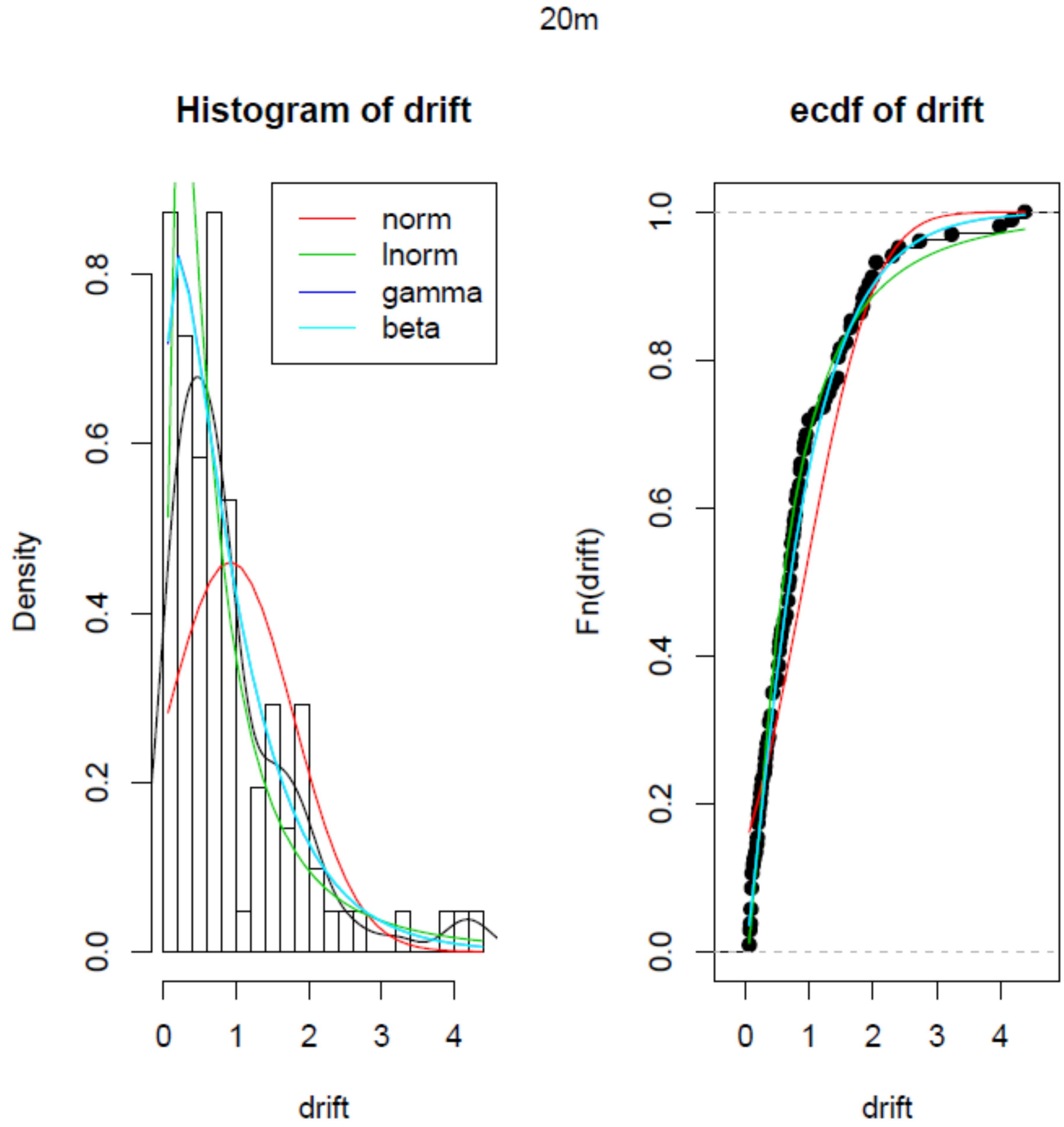


Figure A 9: Illustration of fitted distributions for hops at 20 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

Orchards-late

Table A 7: PDF parameters and statistics, 'Lumped-analysis' – orchards-late.

	3 m	5 m	7.5 m	10 m	15 m	20 m	30 m	50 m
normal								
mean	8.148	4.571	2.742	1.843	0.955	0.557	0.248	NA
sd	5.078	2.740	1.775	1.295	0.731	0.415	0.205	NA
p	0.001	0.006	0.004	0.016	0.029	0.074	0.011	NA
D	0.142	0.125	0.134	0.114	0.106	0.094	0.118	NA
BIC	1118.4	918.11	699.86	634.53	423.84	211.93	-51.525	NA
lognorm								
mean	1.935	1.337	0.772	0.256	-0.475	-0.955	-1.768	NA
sd	0.555	0.629	0.764	1.017	1.145	1.011	0.965	NA
p	0.060	0.756	0.159	0.005	0.003	0.004	0.036	NA
D	0.098	0.049	0.085	0.127	0.131	0.130	0.104	NA
BIC	1017.3	867.60	675.39	639.57	414.08	187.84	-133.16	NA
gamma								
shape	3.235	2.894	2.266	1.551	1.305	1.497	1.483	NA
rate	0.397	0.633	0.827	0.842	1.366	2.688	5.978	NA
p	0.043	0.537	0.450	0.369	0.181	0.287	0.542	NA
D	0.103	0.059	0.065	0.067	0.080	0.072	0.059	NA
BIC	1036.3	863.87	651.98	590.77	359.83	148.98	-152.73	NA
beta								
alpha	2.923	2.767	2.216	1.534	1.299	1.787	1.464	NA
beta	32.797	57.73	78.65	81.82	134.95	319.21	586.24	NA
p	0.046	0.503	0.416	0.393	0.188	0.180	0.560	NA
D	0.102	0.060	0.067	0.066	0.079	0.080	0.058	NA
BIC	1040.9	864.30	651.76	589.97	359.41	NA	NA	NA

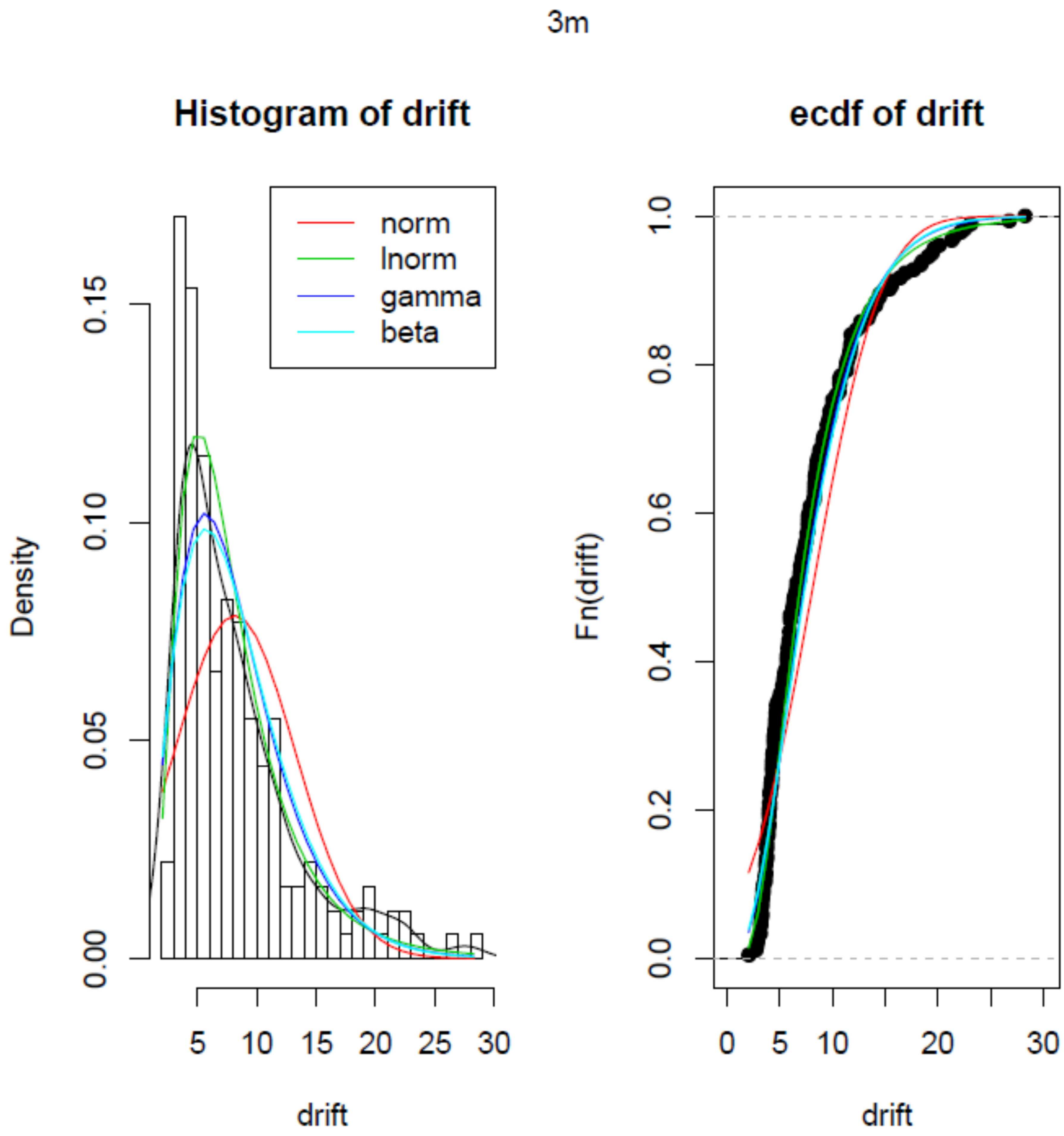


Figure A 10: Illustration of fitted distributions for orchards-late at 3 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

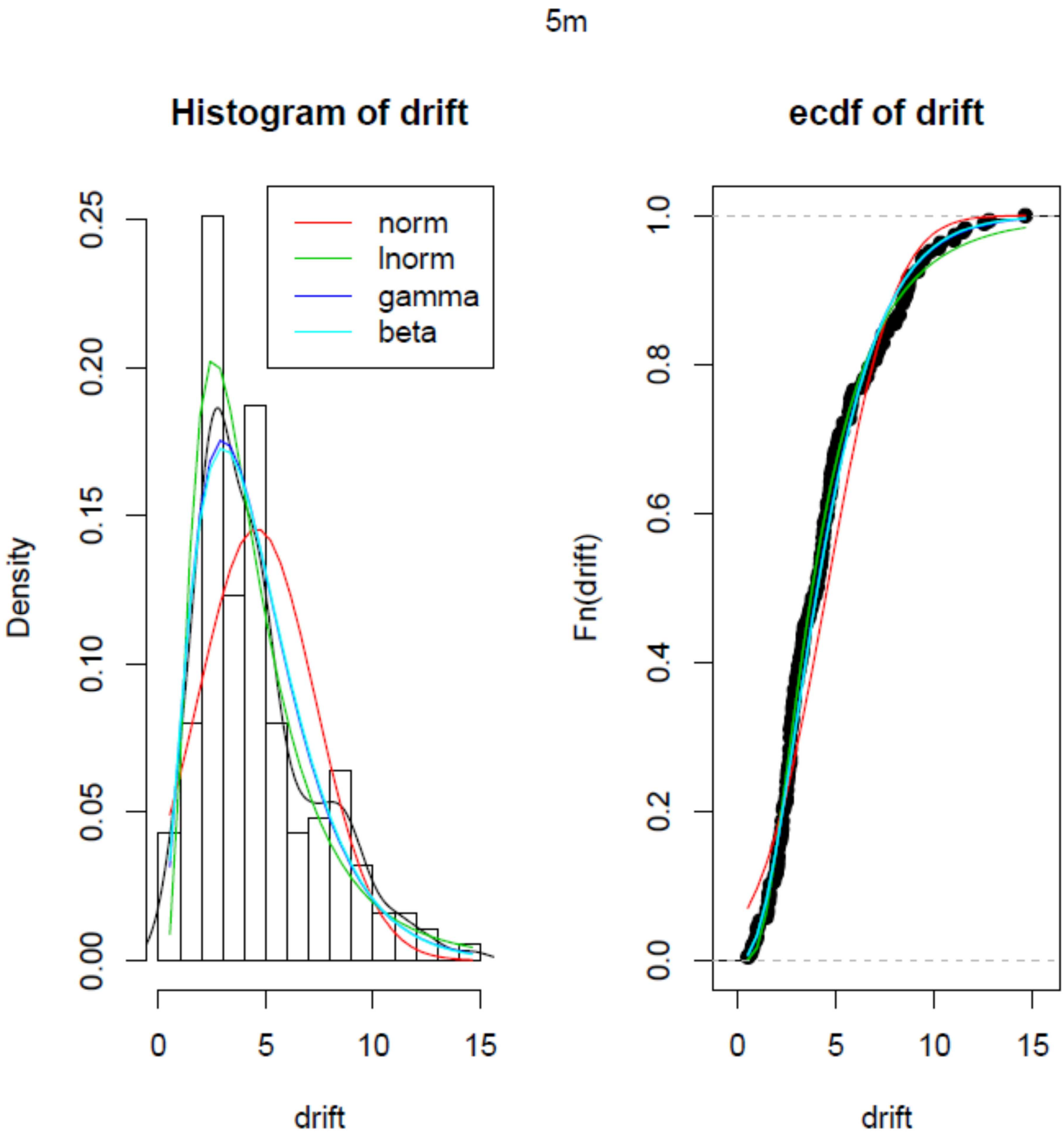


Figure A 11: Illustration of fitted distributions for orchards-late at 5 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

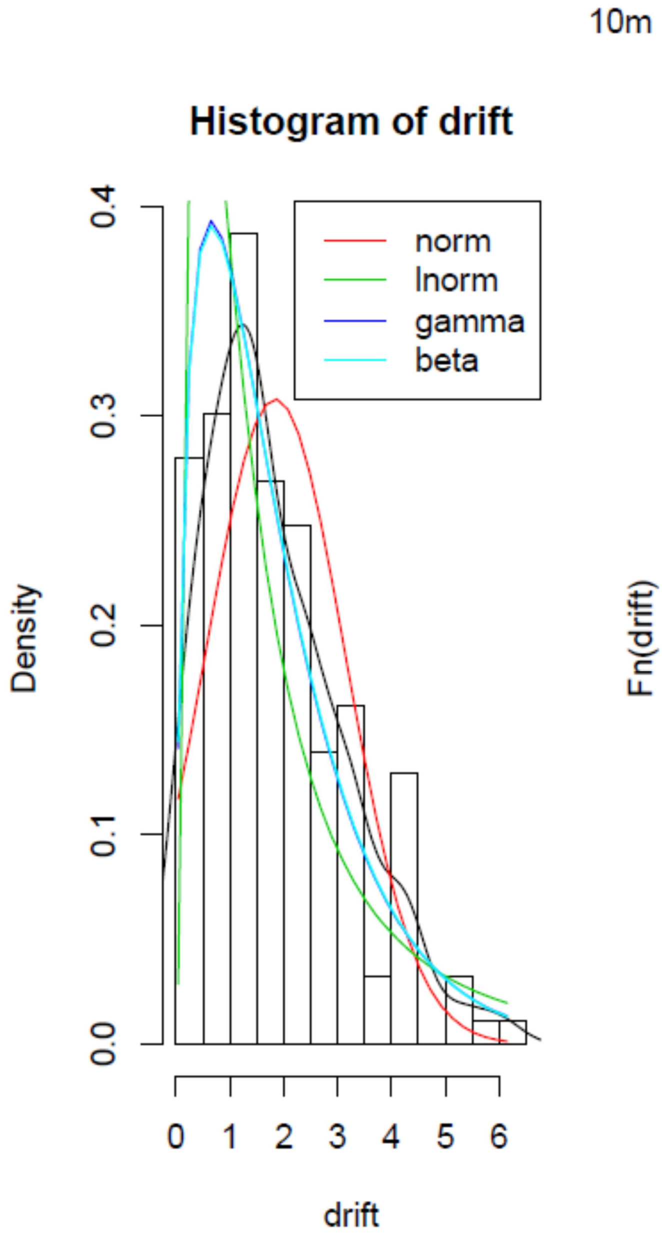


Figure A 12: Illustration of fitted distributions for orchards-late at 10 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

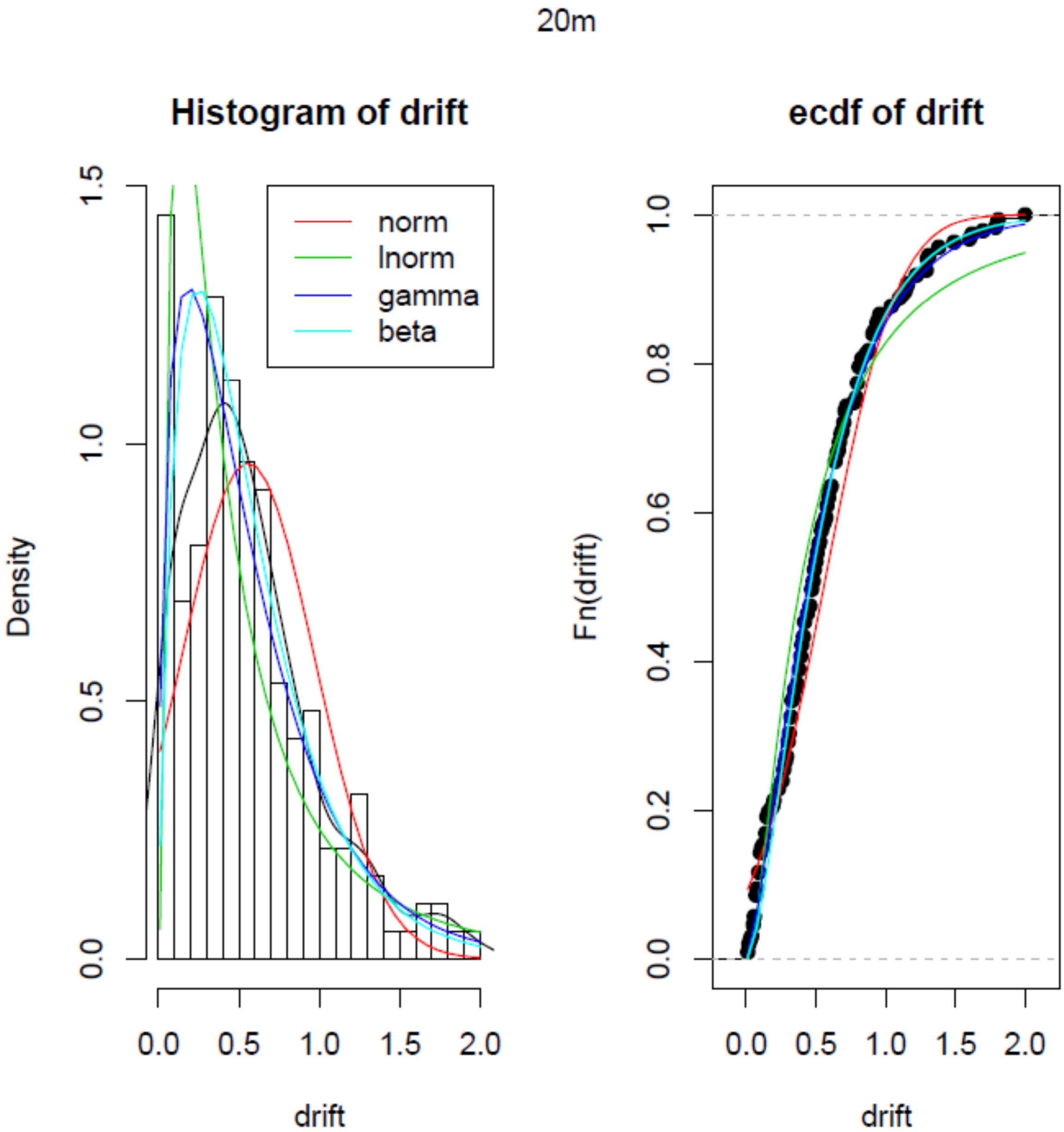


Figure A 13: Illustration of fitted distributions for orchards-late at 20 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

Orchards-early

Table A 8: PDF parameters and statistics, 'Lumped-analysis' – orchards-early.

	3 m	5 m	7.5 m	10 m	15 m	20 m	30 m	50 m	75 m	100 m
normal										
mean	18.098	14.542	8.224	6.250	3.181	1.911	0.860	0.107	0.046	0.027
sd	6.585	8.165	3.624	3.623	2.148	1.251	0.662	0.109	0.040	0.024
p	0.729	0.000	0.661	0.046	0.000	0.031	0.000	0.000	0.007	0.001
D	0.039	0.132	0.041	0.068	0.121	0.071	0.108	0.236	0.167	0.191
BIC	2053	2897	1690	2231	1781	1359	837.3	-388.6	-353.1	-449.5
lognorm										
mean	2.811	2.534	1.961	1.626	0.908	0.341	-0.595	-2.944	-3.479	-4.051
sd	0.458	0.568	0.638	0.729	0.772	0.912	1.172	1.420	0.963	0.961
p	0.011	0.033	0.000	0.005	0.000	0.000	0.000	0.000	0.440	0.334
D	0.092	0.071	0.122	0.086	0.104	0.127	0.146	0.192	0.087	0.094
BIC	2143	2790	1829	2250	1687	1380	817.5	-576.2	-410.4	-525.0
gamma										
shape	6.041	3.649	3.590	2.576	2.160	1.777	1.265	0.830	1.423	1.332
rate	0.334	0.251	0.437	0.412	0.679	0.930	1.471	7.742	31.23	50.28
p	0.244	0.038	0.031	0.305	0.136	0.023	0.004	0.000	0.913	0.393
D	0.058	0.069	0.082	0.048	0.058	0.074	0.087	0.138	0.056	0.090
BIC	2087	2760	1740	2174	1647	1295	695.5	-611.4	-415.4	-521.5
beta										
alpha	5.167	3.018	3.395	2.447	2.099	1.755	1.261	0.969	1.356	1.226
beta	23.46	17.59	38.02	36.76	63.86	90.21	145.5	903.0	2912	4444
p	0.415	0.005	0.052	0.441	0.167	0.029	0.004	0.000	0.827	0.212
D	0.050	0.086	0.077	0.043	0.055	0.072	0.086	0.155	0.063	0.106
BIC	2075	2778	1732	2170	1647	1293	694.6	NA	NA	NA

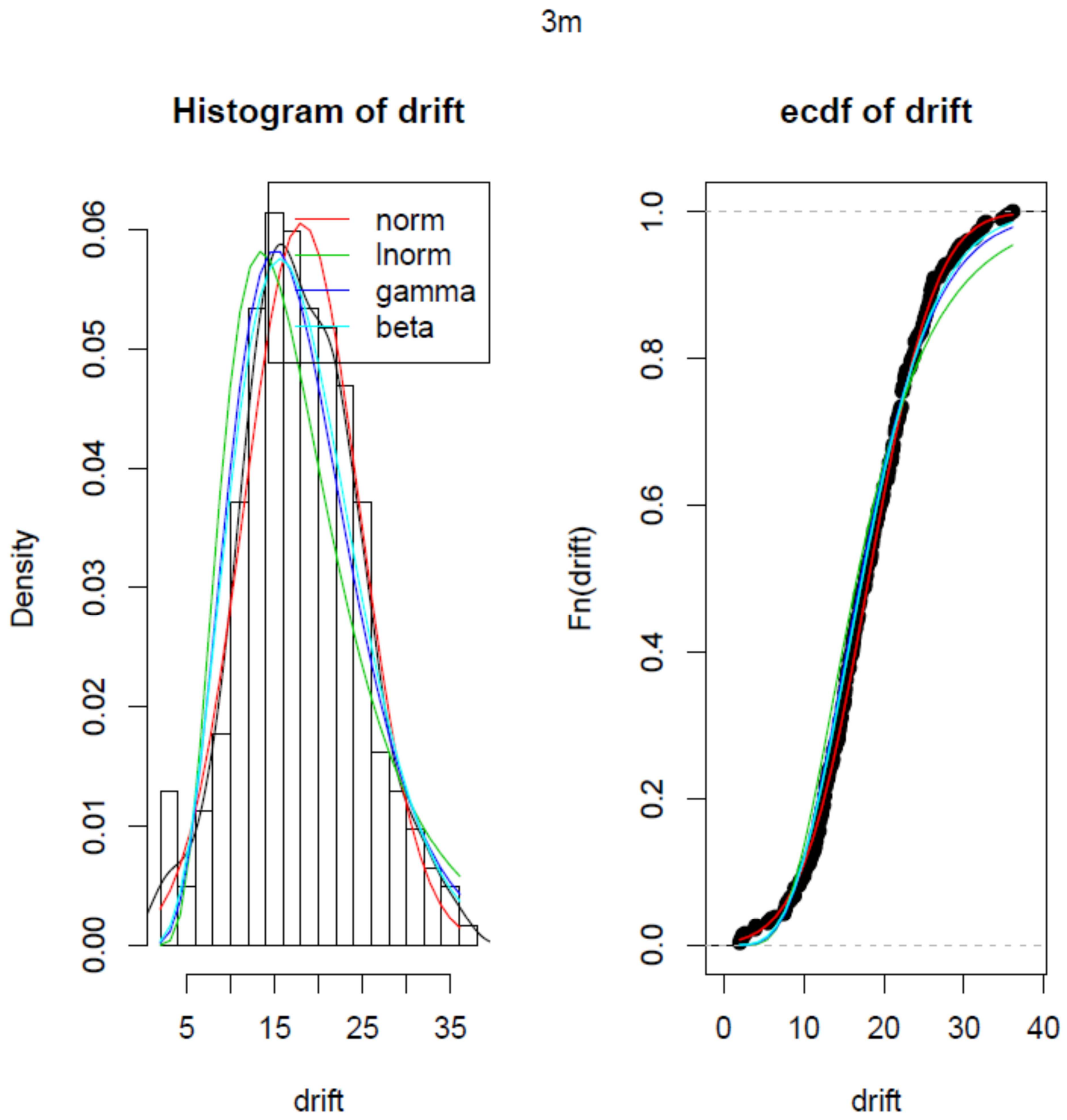


Figure A 14: Illustration of fitted distributions for orchards-early at 3 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

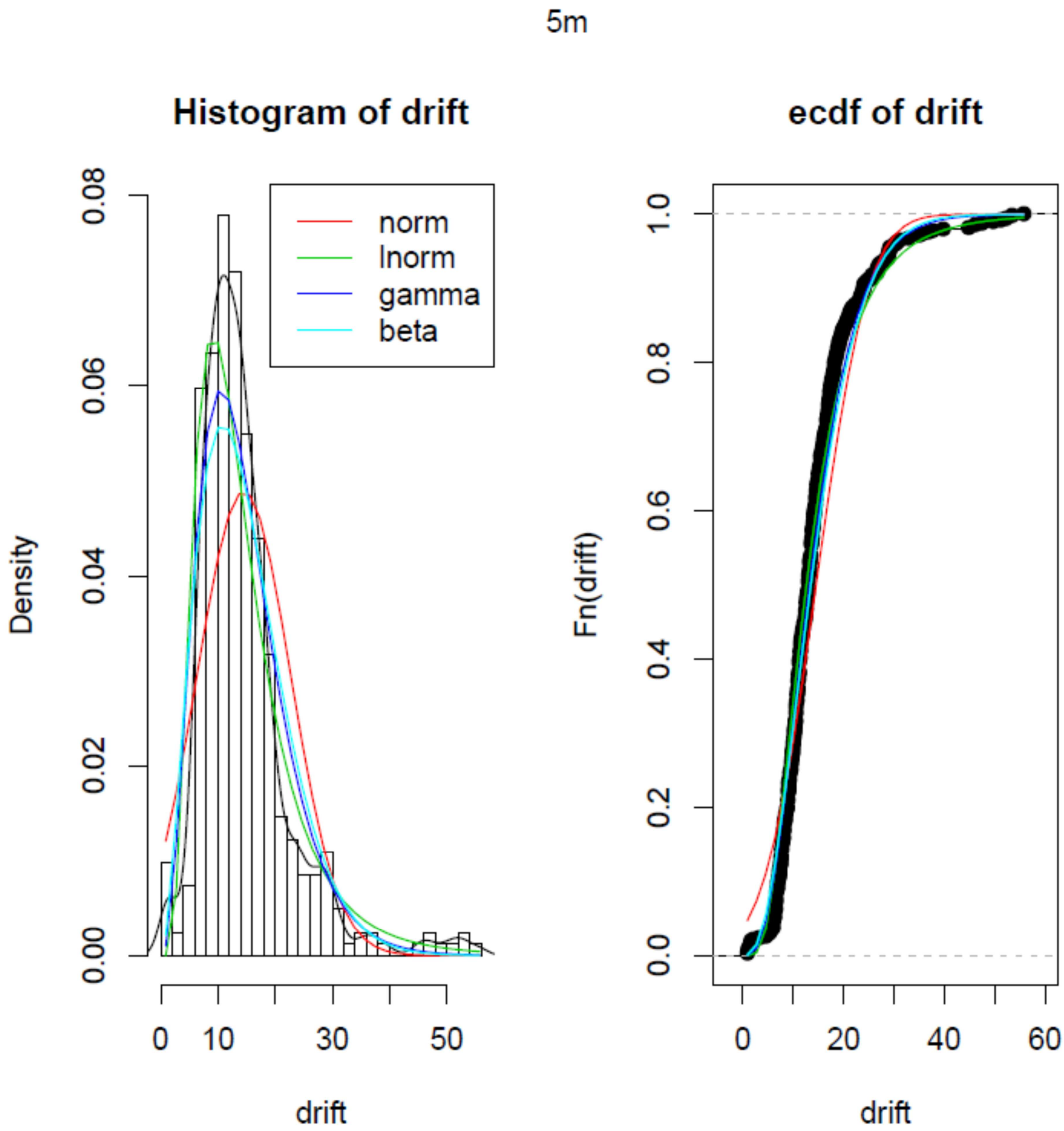


Figure A 15: Illustration of fitted distributions for orchards-early at 5 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

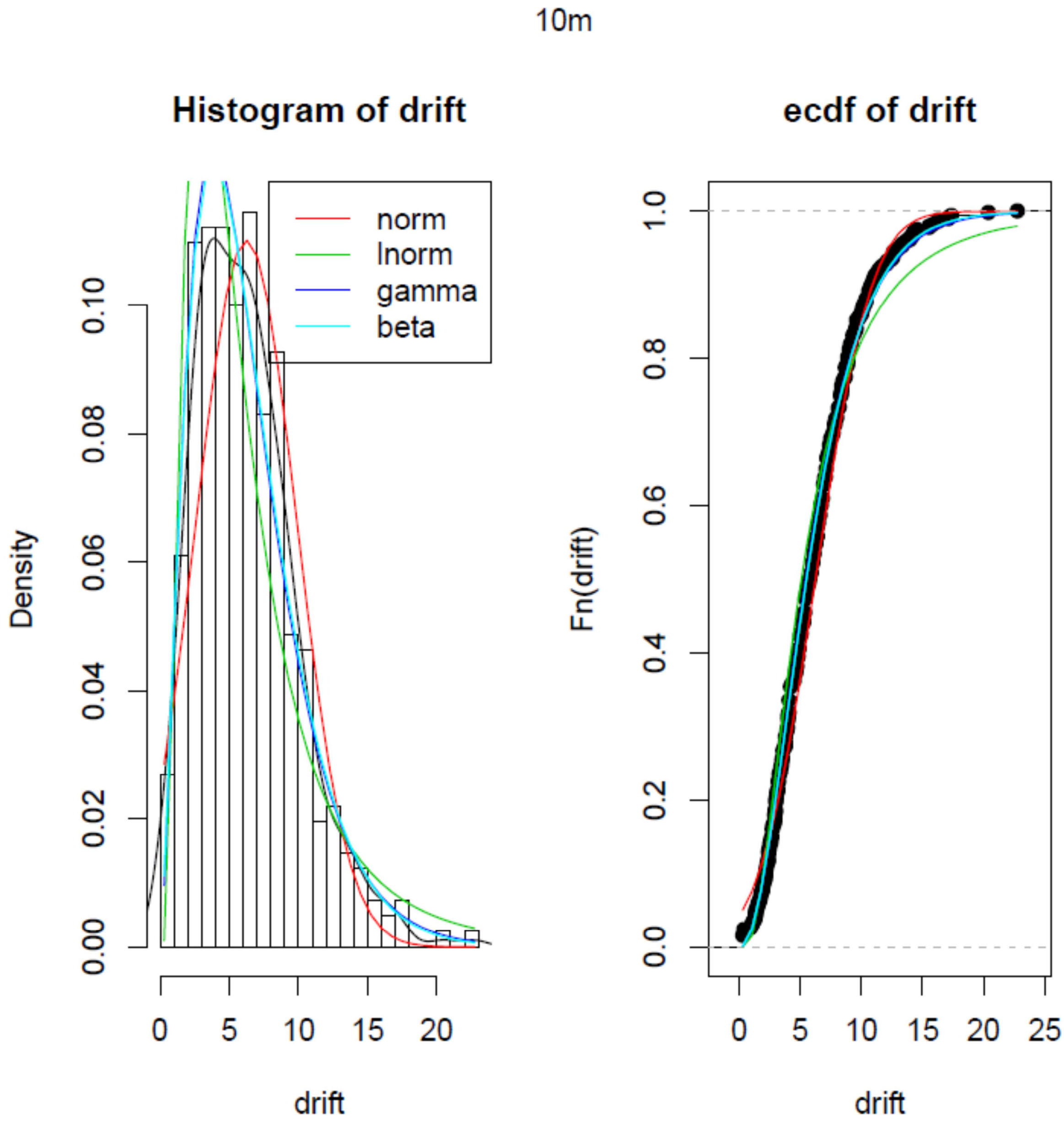


Figure A 16: Illustration of fitted distributions for orchards-early at 10 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

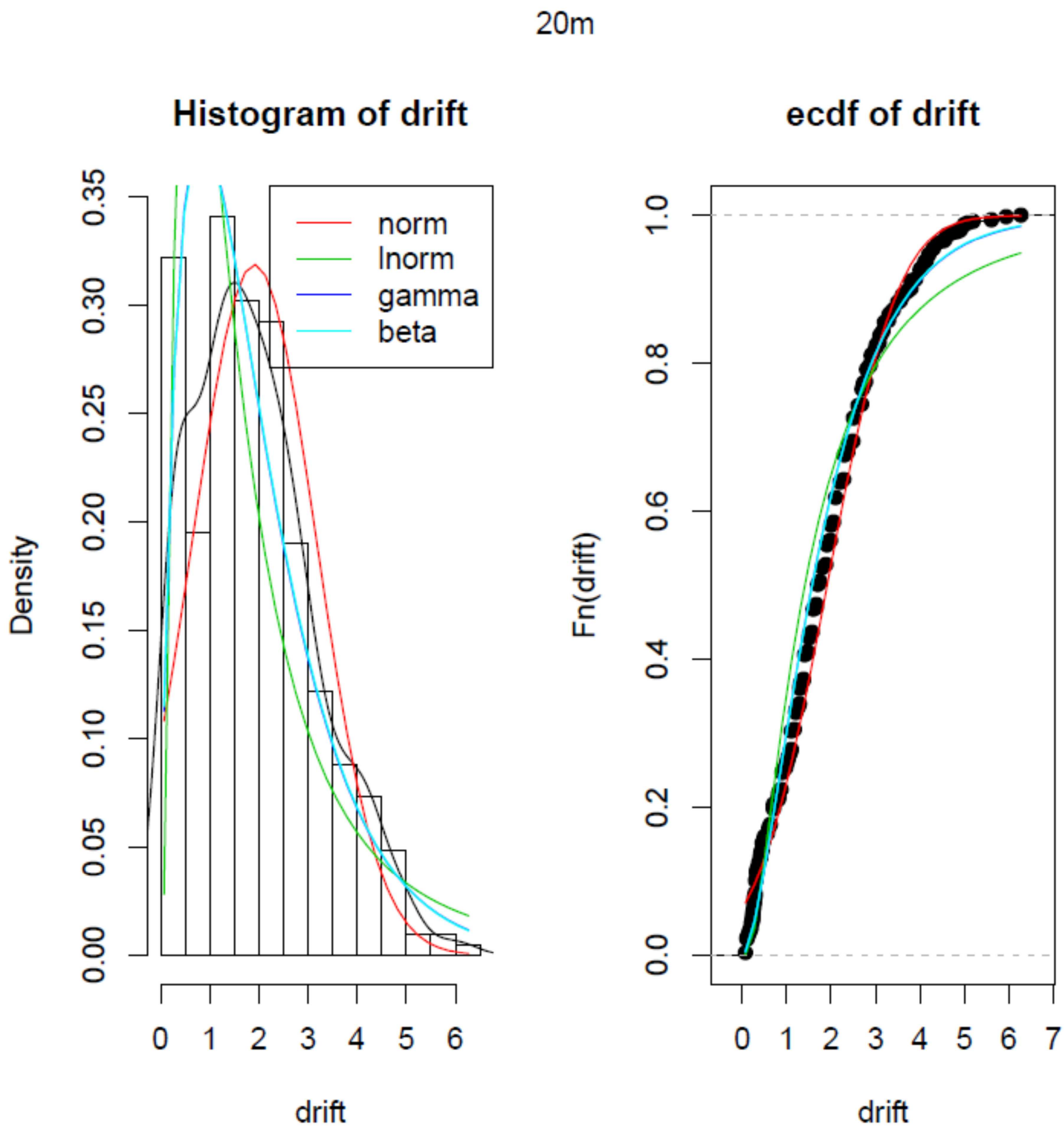


Figure A 17: Illustration of fitted distributions for orchards-early at 20 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

Vines

Table A 9: PDF parameters and statistics, 'Lumped-analysis' – vines.

	3 m	5 m	7.5 m	10 m	15 m	20 m	30 m	50 m
normal								
mean	3.849	1.847	1.014	0.621	0.286	0.159	0.017	0.030
sd	1.910	1.314	0.723	0.479	0.226	0.117	0.017	0.036
p	0.206	0.004	0.016	0.006	0.005	0.000	0.000	0.002
D	0.087	0.144	0.127	0.140	0.142	0.174	0.308	0.243
BIC	625.75	514.21	336.02	213.47	-10.475	-206.64	-614.99	-216.26
lognorm								
mean	1.191	0.307	-0.303	-0.844	-1.589	-2.135	-4.541	-4.101
sd	0.612	0.855	0.868	0.967	0.884	0.809	0.923	1.088
p	0.126	0.291	0.034	0.031	0.186	0.571	0.000	0.015
D	0.096	0.080	0.117	0.118	0.089	0.064	0.336	0.203
BIC	641.68	477.66	300.31	171.22	-77.51	-266.47	-746.24	-298.40
gamma								
shape	3.352	1.781	1.725	1.506	1.621	1.844	1.229	0.965
rate	0.871	0.964	1.701	2.426	5.659	11.611	72.797	31.969
p	0.186	0.444	0.262	0.362	0.206	0.166	0.000	0.016
D	0.089	0.071	0.083	0.076	0.087	0.091	0.330	0.202
BIC	622.38	465.85	289.48	152.42	-82.79	-268.14	-720.93	-287.00
beta								
alpha	3.254	1.759	1.939	1.663	1.605	1.839	1.053	0.697
beta	81.38	93.58	189.28	266.28	557.12	1156.16	5725.4	2309.3
p	0.199	0.453	0.291	0.339	0.210	0.165	0.000	0.003
D	0.088	0.070	0.080	0.077	0.087	0.091	0.316	0.233
BIC	621.35	465.57	NA	NA	NA	NA	NA	NA

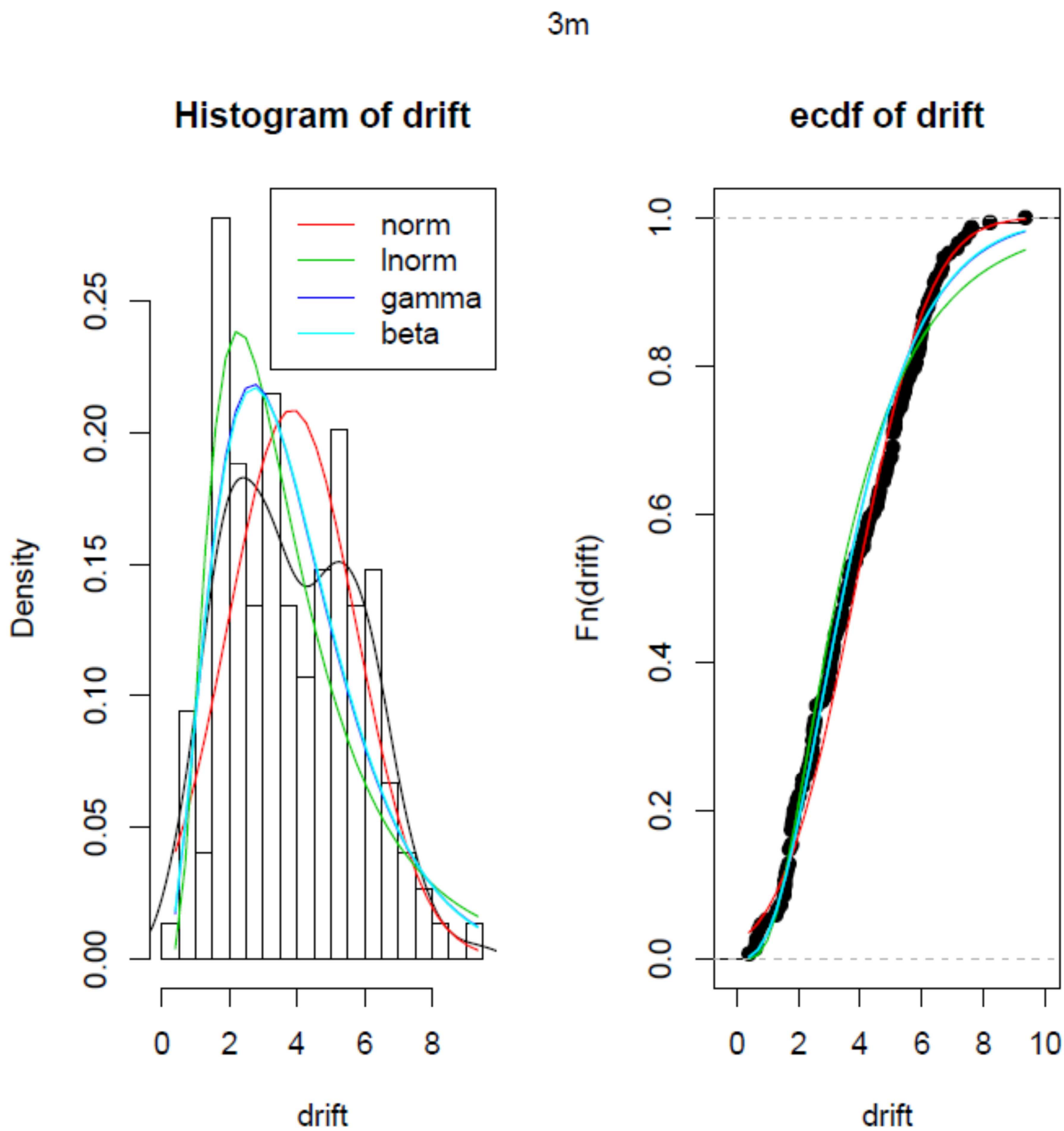


Figure A 18: Illustration of fitted distributions for vines at 3 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

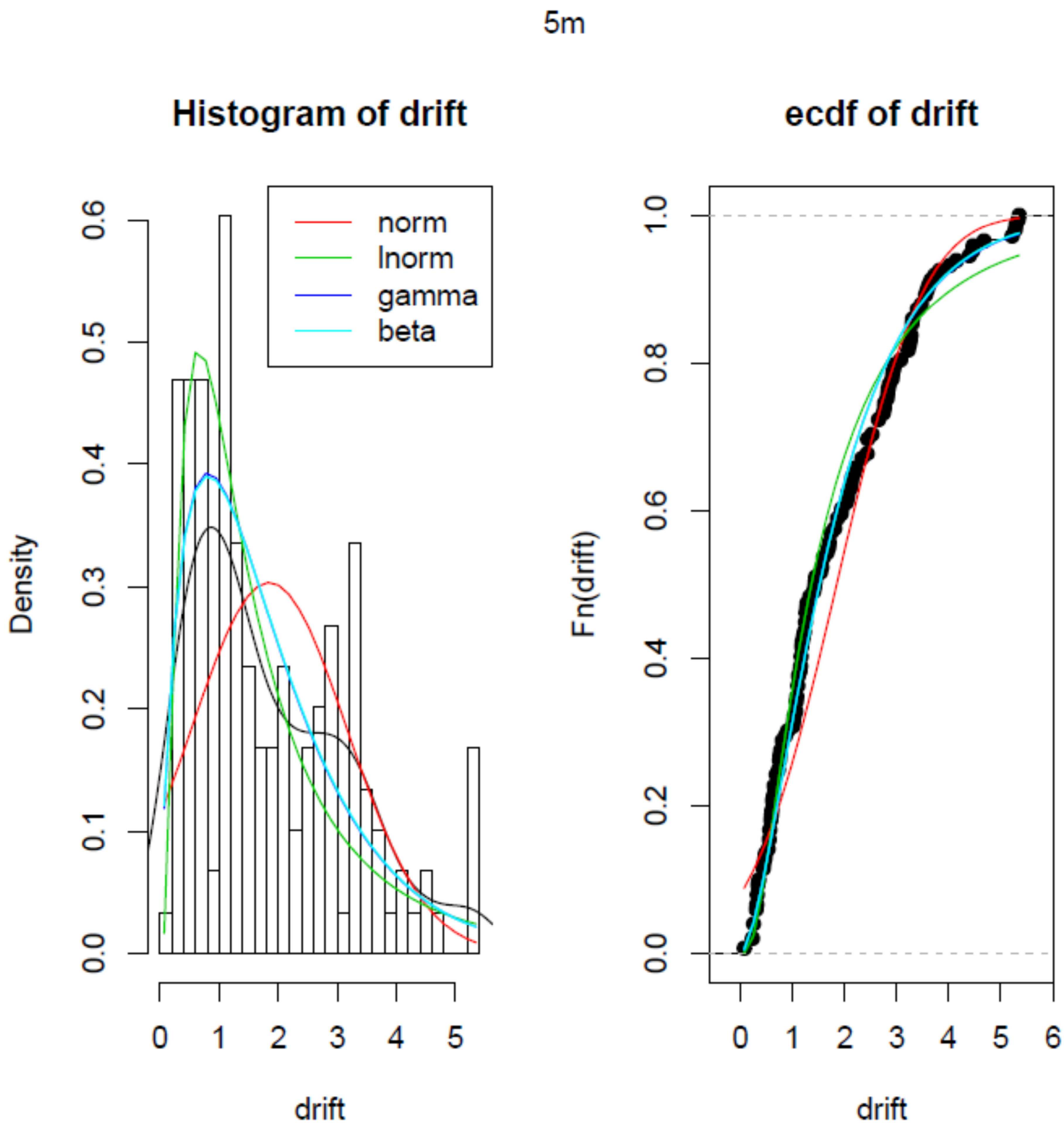


Figure A 19: Illustration of fitted distributions for vines at 5 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

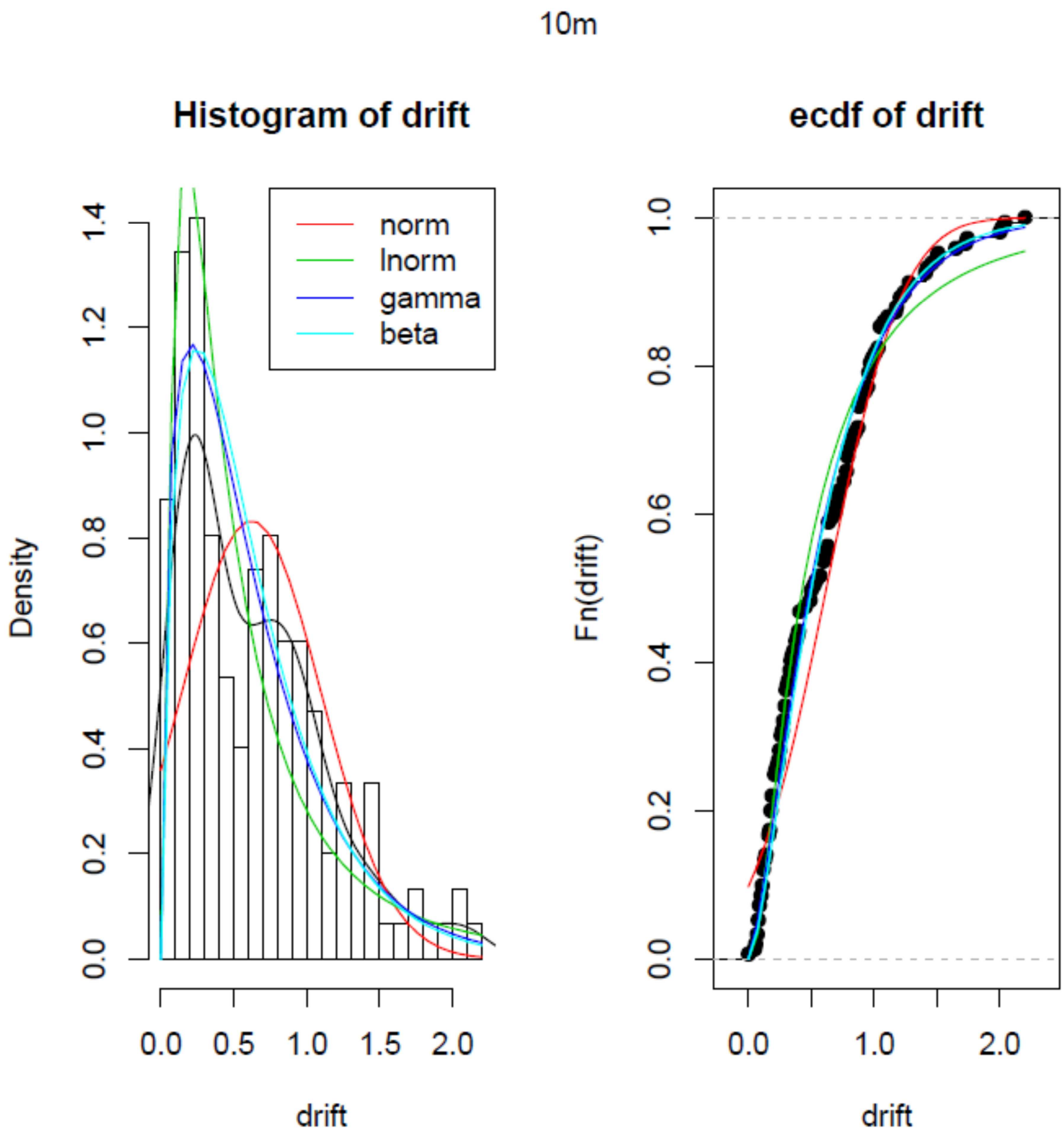


Figure A 20: Illustration of fitted distributions for vines at 10 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

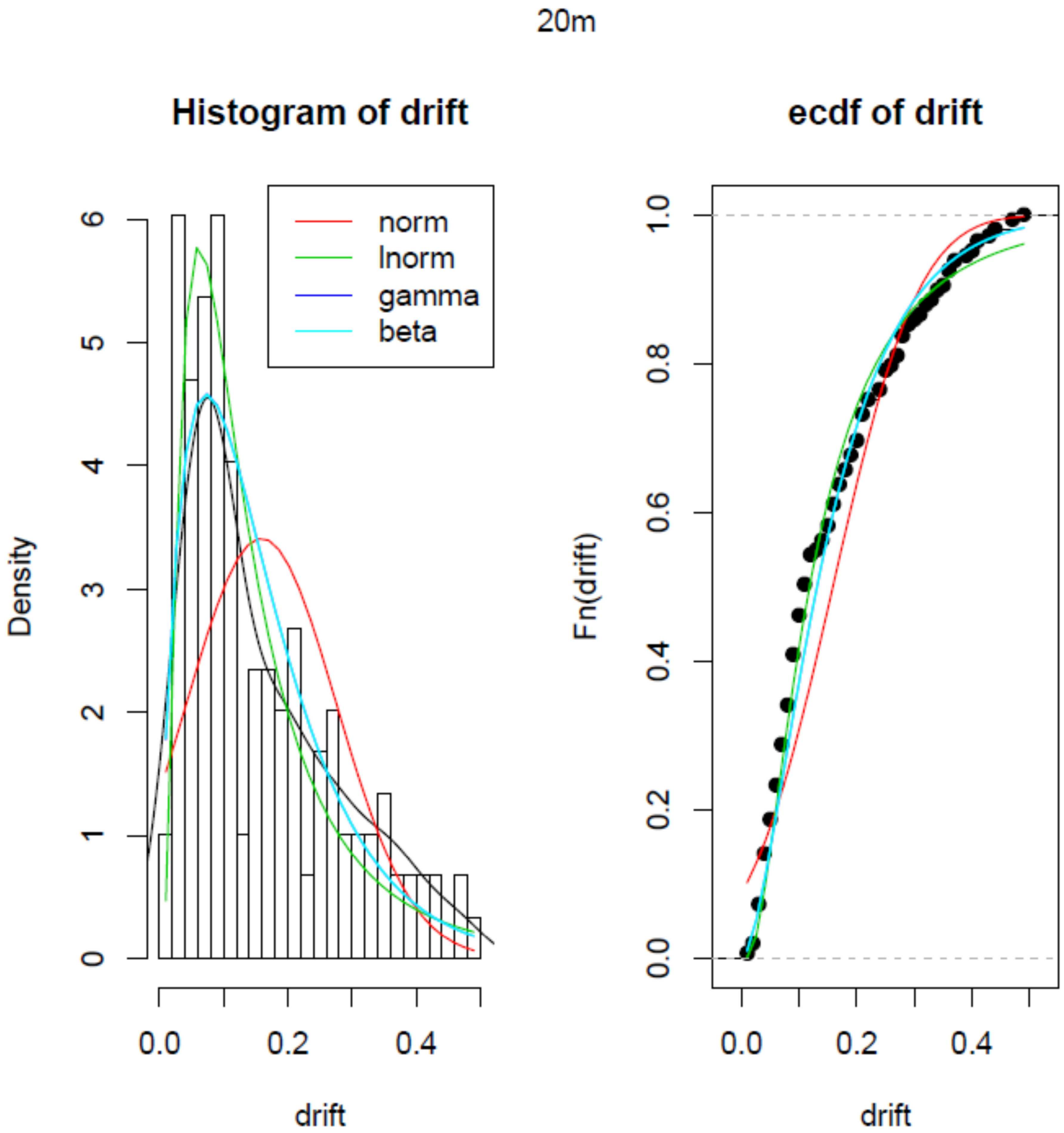
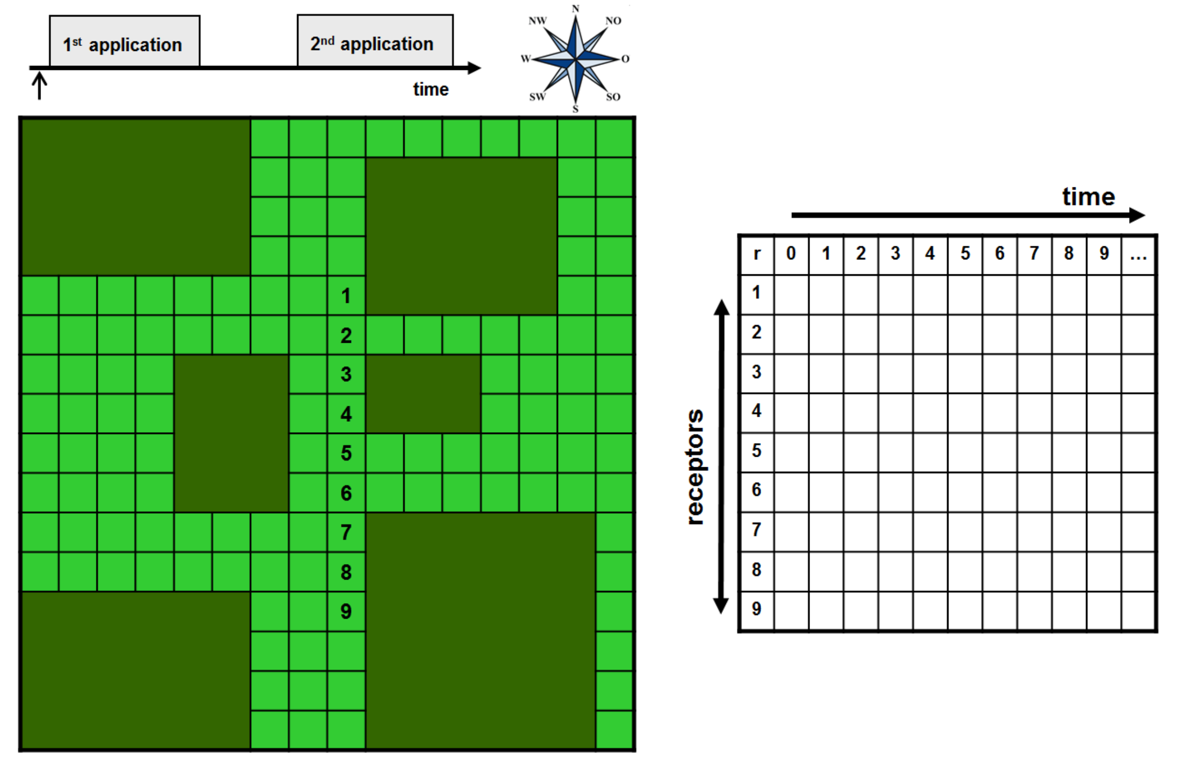


Figure A 21: Illustration of fitted distributions for vines at 20 m distance. Histogram of the drift data is plotted along with four fitted distributions in the left panel. The plot shows how close (or how far) the best fitting probability densities of the four distributions approximate the non-parametric probability density estimate (black line). The empirical CDF ('ecdf') is plotted along with the CDF of the fitted distribution in the right panel.

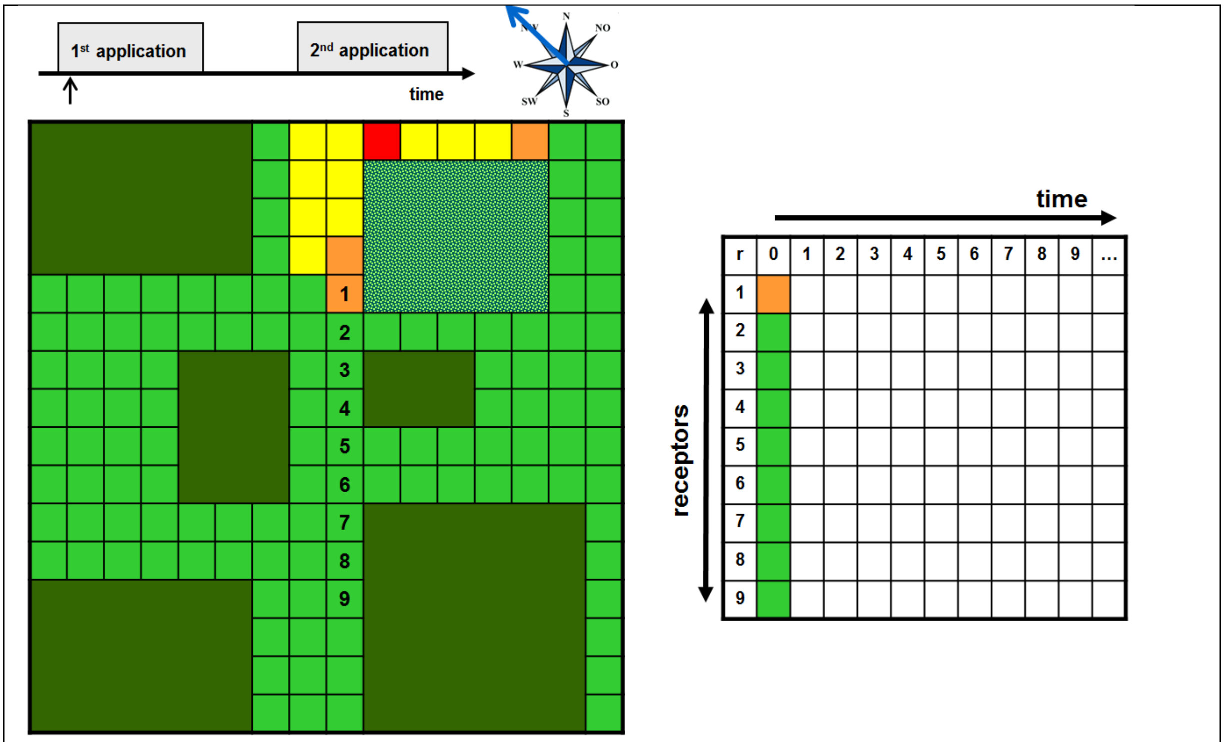
11.4 Simulation Process: Schematic Generation of PEC(r,t)-Matrix

Figure A 22 (this and following pages) illustrates the generation of a PEC(r,t) matrix.

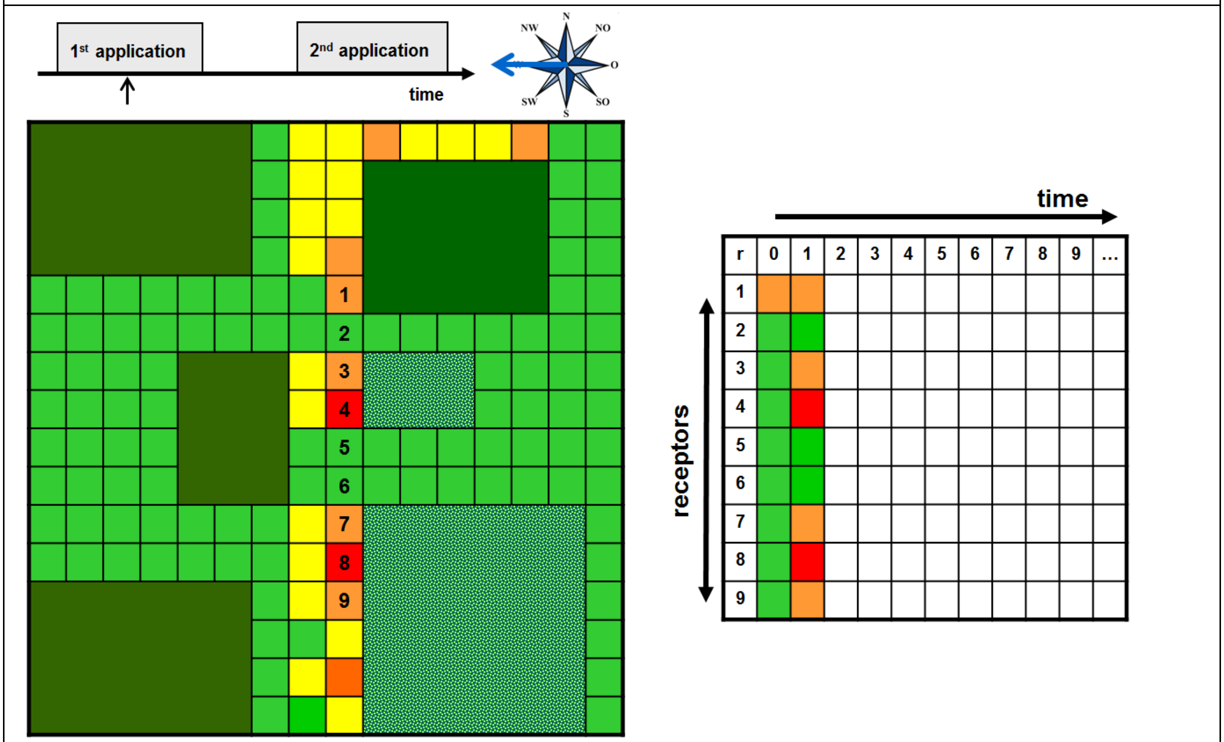
Figure A 22: Illustration of PEC(r,t) matrix generation. Exposure due to spray-drift, taking dissipation of the substance into account (upper left diagram: simulation time progress; upper right: current wind direction; central left: landscape; right: PEC(r,t)-matrix) (landscape: dark green rectangles: fields (currently no application), light green rectangles: fields (application in this time-step); small grid cells: *Off-Crop-Receptors*, cells '1-9': exemplarily assessed *Off-Crop-Receptors*, light green, yellow, orange, red cells indicate increasing exposure level.)



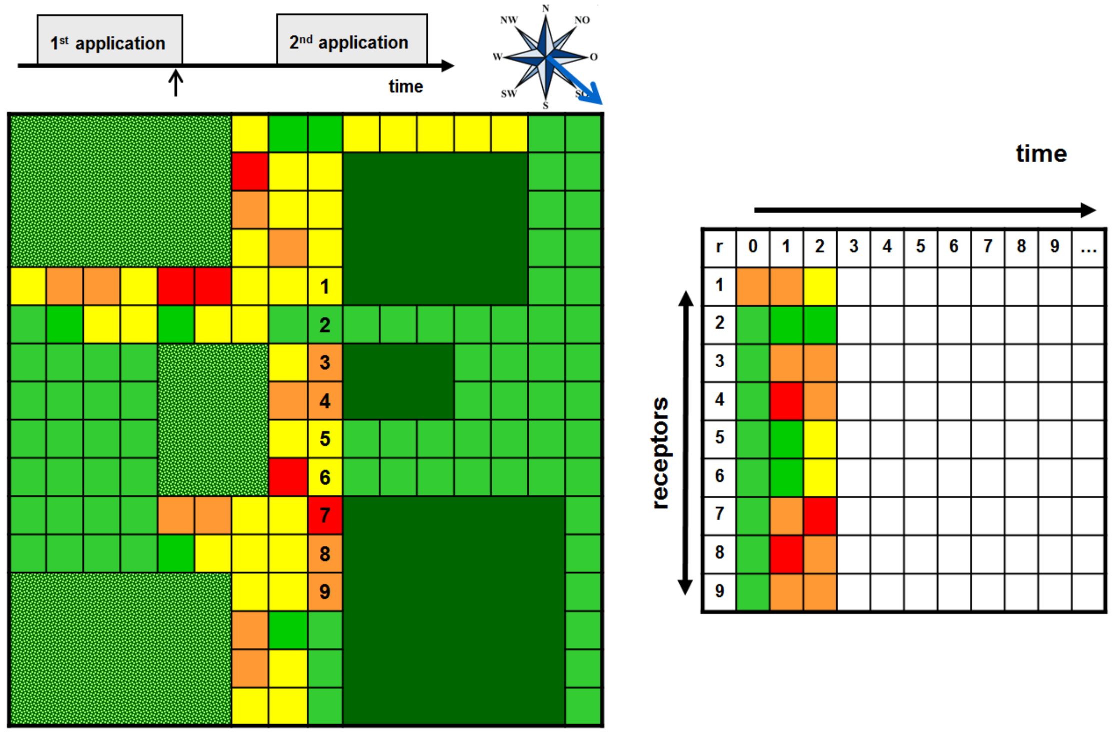
$t<t_0$: no application has happend yet.



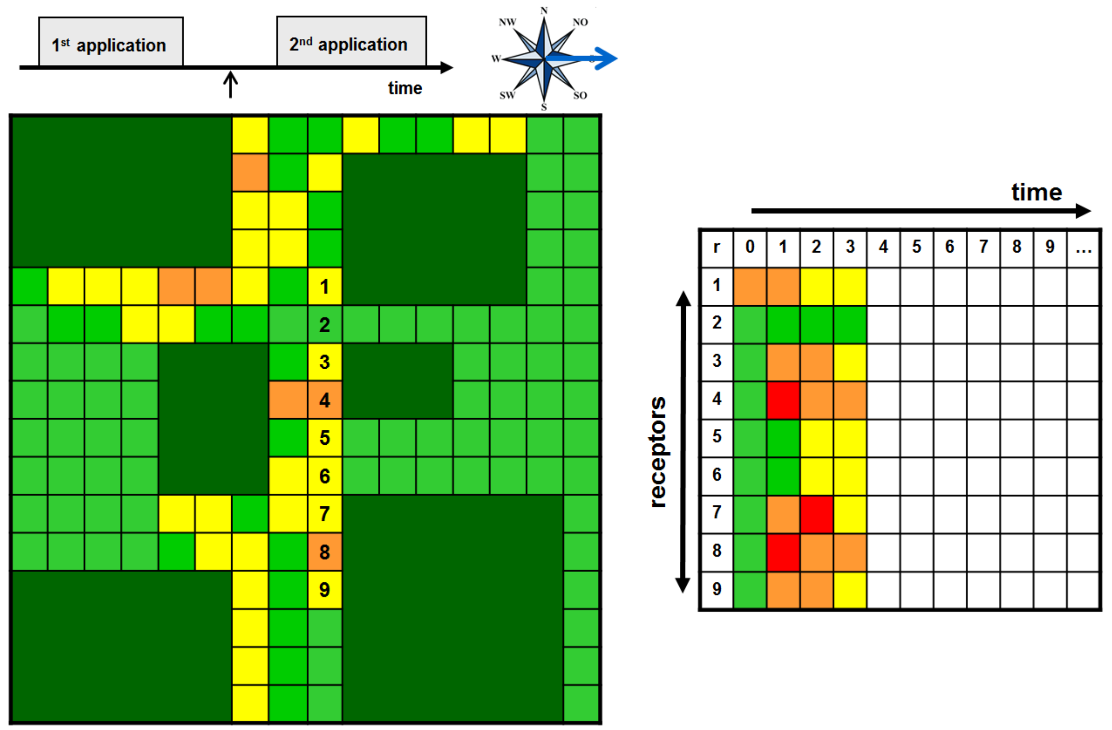
t_0: 1st application at north-east right field; south-eastern wind direction; spray-drift deposition downwind (variable).



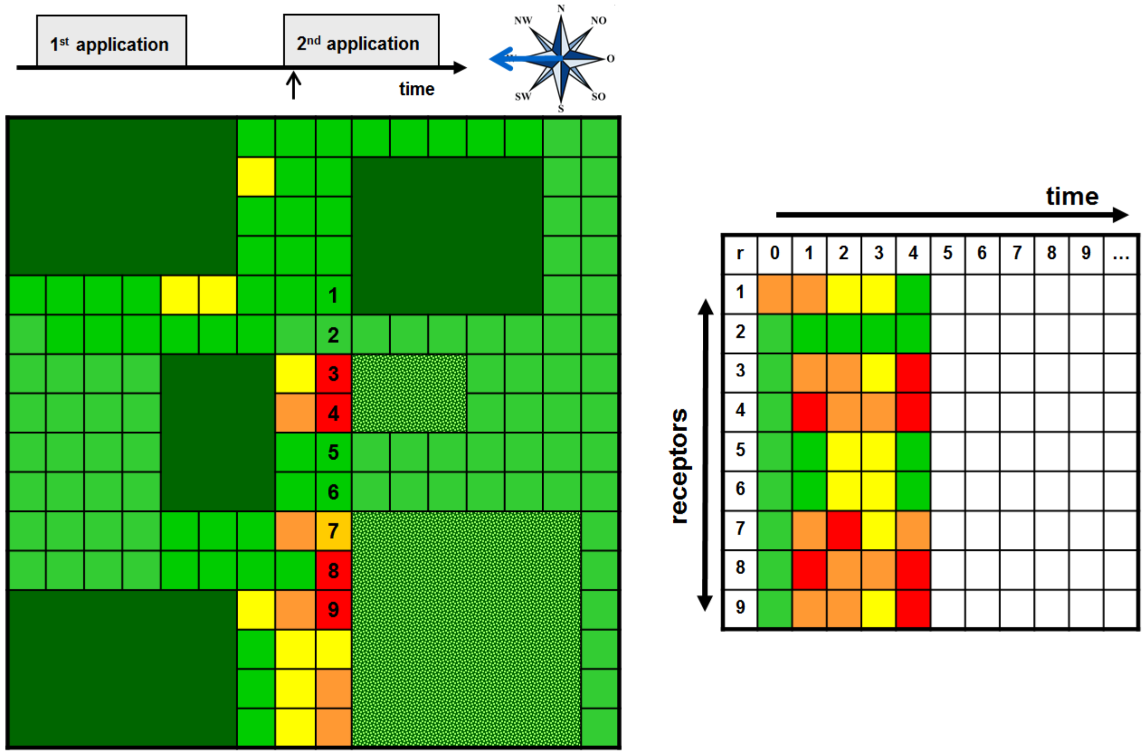
t_1: 1st application at central east and south-east fields; eastern wind direction; spray-drift deposition downwind (variable).



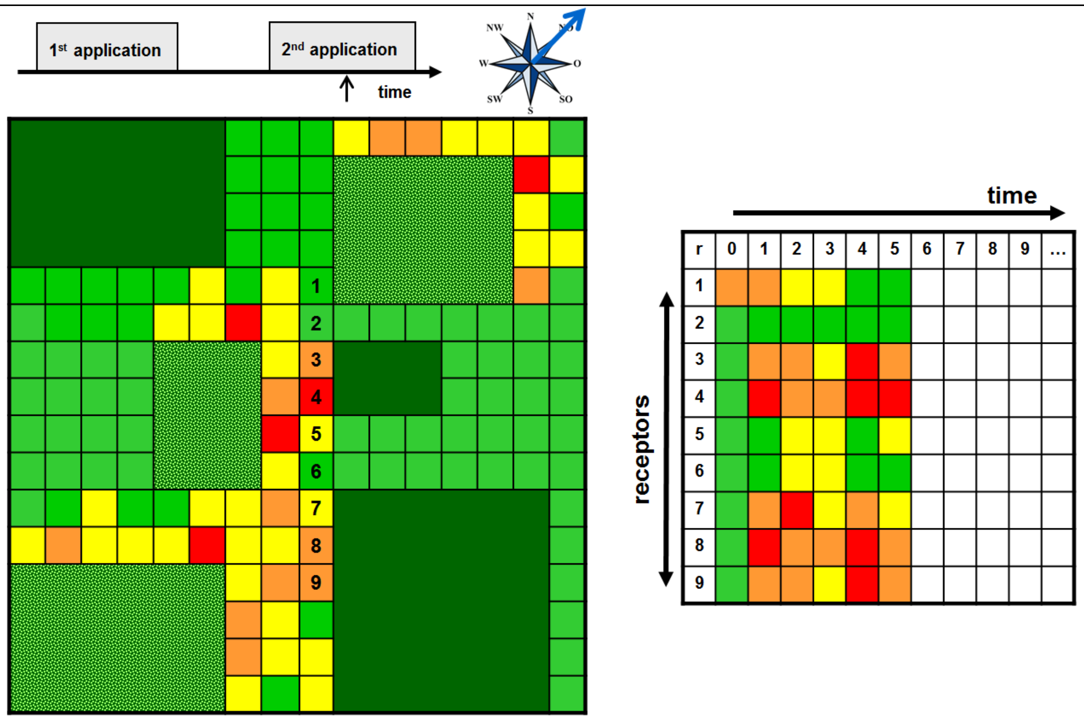
t$_2$: 1st application at western fields; north-western wind direction; spray-drift deposition downwind (variable).



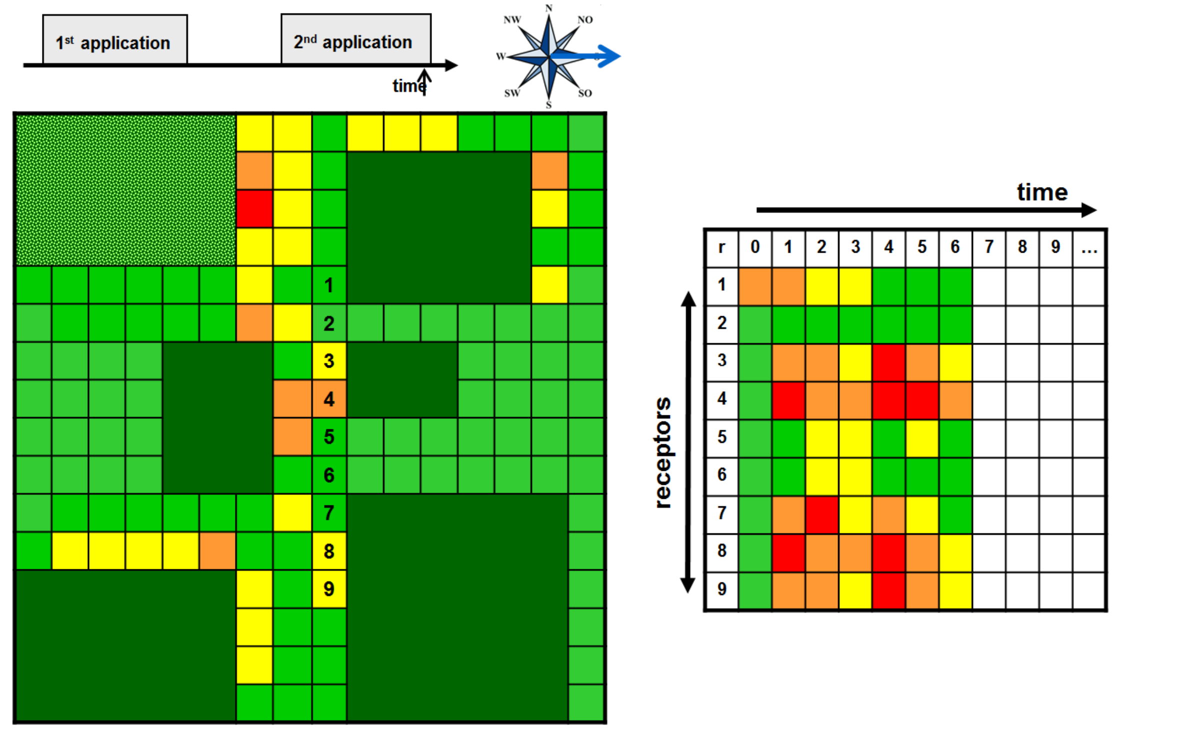
t$_3$: no application; western wind direction; no spray-drift deposition.



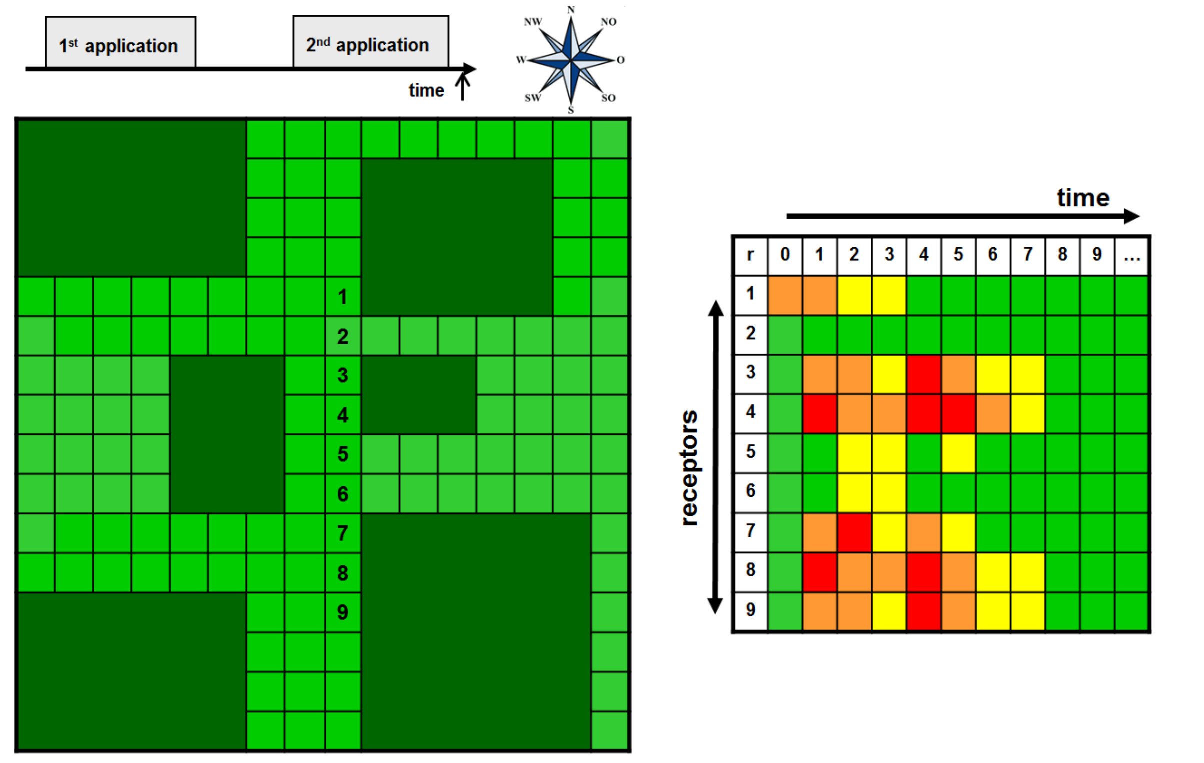
t_4: 2nd application at central- and south-eastern fields; eastern wind direction; spray-drift deposition downwind (variable).



t_5: 2nd application at central- and south-western, as well as north-eastern fields; south-western wind direction; spray-drift deposition downwind (variable).



t_6: 2nd application at north-western field; western wind direction; spray-drift deposition downwind (variable).



t_7: no application; no spray-drift deposition.

12 Curriculum Vitae

Personal Information
Date of Birth 26 July 1966
Place of Birth Laubach (Germany)
Citizenship German
Address Bern 23a, 42799 Leichlingen

Education
School
1972 to 1974 Primary school "Grundschule Laubach-Wetterfeld"
1974 to 1976 Primary school "Grundschule Laubach"
1976 to 1982 Intermediate School "Gesamtschule Laubach"
1982 to 1983 Secondary school Fachoberschule "Theodor-Litt Schule Giessen"
1983 to 1986 Secondary school Gymnasium "Laubach-Kolleg der Evangelischen Kirche in Hessen und Nassau", Degree "Abitur"

University
1986 to 1996 Study of Physics and Biology at the "University Giessen"
1989 Intermediate Diploma in Physics
1990 Diploma examination in minor subject Mathematics
1991 Main mandatory internship (Physics)
1993 Intermediate Diploma in Biology
1995 to 1996 "Helmholtz Centre for Environmental Research (UFZ) Leipzig-Halle, Dept. Ecosystem Analysis/Ecological Modelling"
1996 Diploma in Biology

Professional Career
1996 to 1997 Research associate at the "University Marburg" (Nature Conservation)
Since 1998 employee at Bayer CropScience

Working Groups
ECPA "GIS Working Group" (European Crop Protection Association)
FOCUS "Landscape And Mitigation Working Group" (Forum for the Co-ordination of pesticide fate models and their Use)
IVA "GeoPERA Working Group" (Industrieverband Agrar)
BVL Panel "Leitungsgremium zur Einführung Probabilistischer Expositionsabschätzungen und neuer Anwendungsbeschränkungen" (Bundesamt für Verbraucherschutz und Lebensmittelsicherheit)
UBA Advisory Board "GeoRisk" (Umweltbundesamt)
SETAC Europe Advisory Group "MeMoRisk" (Society of Environmental Toxicology and Chemistry)
SETAC Europe Workshops "LEMTOX", "MODELINK"

13 Erklärung

Erklärung über Anteile von Koautoren sowie benutzte Hilfsmittel in der vorgelegten Dissertation.

Das Projekt 'Xplicit', in dessen Kontext die genannte Dissertation angefertigt wurde, hat seit seiner Initiierung (die selbst eine eigene Leistung darstellt) einen fachlich-wissenschaftlichen, als auch methodisch-technischen Umfang und Detailreichtum angenommen, welche die Kooperation mit Kollegen und Instituten selbstverständlich machte. Nachfolgend sind meine persönlichen Leistungen sowie die Beiträge von Kollegen in dieser Kooperation meiner Dissertation dargestellt. Vermerke zu den Beiträgen der Koautoren finden sich auch an entsprechenden Textstellen der Dissertation (auch in 'Acknowledgements', Section 9).

Die Motivation zur Entwicklung von 'Xplicit' ist eine persönliche Leistung und begründet sich auf eigene Studien und Vorarbeiten, meinen Beiträgen zu Projekten wie z.B. FOCUS Landscape & Mitigation (FOCUS 2007a, 2007b) oder GeoPERA (z.B. Schad et al. 2007), der Teilnahme an und Beiträgen zu Konferenzen und Workshops sowie der Literatur-Recherche. Damit wurde die Grundlage für den Rahmen und die allgemeinen Ziele zur Entwicklung von 'Xplicit' etabliert, ein Teilabschnitt, der ebenfalls persönliche Leistung darstellt ('Part-1' der Dissertation). Dazu gehörte auch diese Ziele an aktuelle wissenschaftliche und regulatorische Entwicklungen anzupassen (z.B. EFSA 2010a). In diese Erörterungen eingeflossen ist insbesondere der Austausch mit Prof. R Schulz, etwa zur ökotoxikologischen Effekt-Charakterisierung, zu ökologischen Bewertungsendpunkten und zu Risiko-Management Konzepten, woraus auch eine frühe Fallstudie resultierte (Schad & Schulz 2011).

Mit der eigentlichen Entwicklung des Models 'Xplicit' habe ich einen Exkurs in Methoden der Software-Entwicklung durchgeführt, mit dem Ziel, das Vorhaben zu strukturieren und seine Komplexität beherrschbar zu halten. Dabei habe ich etablierte Verfahren der Softwareentwicklung an die Gegebenheiten der wissenschaftlichen Modell-Entwicklung adaptiert (Section 5.2). Auf dieser Basis, habe ich die eigentliche Entwicklung des *Xplicit-Framework* in Anforderungsanalyse, Architektur-Entwurf, System Design, und Implementierung gegliedert. In der ersten Modellversion sind sämtliche Arbeitsschritte von mir selbst umgesetzt worden, was auch für die Programmierung gilt ('Implementierung'). Mit wachsendem Umfang der Software sowie der Komplexität der Module wurde die Programmierung von Kollegen unterstützt und übernommen (insbesondere durch S Bub, siehe 'Acknowledgements', Section 9). Dabei wurde die Definition der Software-Architektur (z.B. Modularität und Service-Orientierung) sowie das System Design weiterhin von mir geleitet und gestaltet, wobei Herr Bub mit wachsender Erfahrung und Kompetenz auch an diesen Stellen sehr wertvolle Beiträge geleistet hat.

Zu den weiteren Bestandteilen (Module, 'Associated Models') des *Xplicit-Framework* sowie der *Xplicit-Models*:

- Grundsätzlich gilt, dass die Motivation, der konzeptionelle Rahmen, die Anforderungen und die Architektur der entwickelten Systeme meine Leistungen darstellen. Dies gilt meist auch für die initiale Implementierung, zu der im Verlauf der Entwicklung, Anwendung und Reifung die genannten Kollegen beigetragen haben oder durch diese übernommen wurde.

- 'Landscape-Metric' (Section 5.3.5.2): Die Idee zur 'Service-Orientierung', die Konzepte, die Architektur und das Design sind meine Leistung, ebenso die initiale Programmierung und Gestaltung der GIS-Prozesse. Im Laufe der Entwicklung wurden die einzelnen Elemente technisch überarbeitet und erweitert (Software, GIS-Module), wozu S Bub und J Wissing wesentlich beigetragen haben.
- 'Schad & Gao Approach' (Section 5.3.5.4): Die Motivation zur statistischen Auswertung der Abdrift-Messungen, das grundsätzliche Design dieser (z.B., 'Individual', 'Lumped', 'A priori Grouping') sowie die Daten-Beschaffung und -Vorbereitung und die initiale statistische Analyse stellen eigene Leistungen dar. Dies gilt auch für die Darstellung der Problematik der skalenabhängigen Variabilität der Abdrift-Deposition. Die finale statistische Auswertung der einzelnen Arbeitsmodule wurde in enger Zusammenarbeit von Z Gao und mir durchgeführt. Der Vorschlag zum 'Mixed-Effect-Model' und die entsprechende Analyse sind persönliche Leistungen von Z Gao.
- 'Spray-drift Filtering by Riparian Vegetation' (Section 5.3.5.5): Die grundsätzliche Idee, Abdrift-Filterung in der Expositionsabschätzung zu berücksichtigen ist nicht neu, wie auch im Text dargestellt. Der wesentliche Punkt meiner persönlichen Leistung hier war, die Angaben in der Literatur mit den Zielen von Xplicit und den typischerweise verfügbaren Geodaten konkret abzustimmen und damit in einem räumlich-zeitlich expliziten Ansatz (Xplicit) instrumentalisierbar zu machen. Dabei habe ich die existierenden Literatur-Recherchen wiederholt und erweitert, wozu auch R Ohliger beigetragen hat. Die Ziele, die Auswertung und die Darstellung der Resultate wurden mit Prof. R Schulz diskutiert.
- 'Recolonisation Potential of Habitat Segments - Xplicit-Distance' (Section 5.3.5.6): Die Idee zu diesem 'Service', die Konzepte, sowie die Architektur und das grundsätzliche Design sind meine Leistung, wobei die Kollegen R Vamshi und C Holmes zum System-Design wesentlich beigetragen haben. Kollege R Vamshi hat die Programmierung umgesetzt, wobei ich zum Design der Klassen und deren Testung beigetragen habe. Die technischen Details der GIS-Prozesse wurden gemeinsam von R Vamshi, C Holmes und mir entwickelt. Der 'Service' wurde von mir in einer Fallstudie (Case Study 'Section 6.1') angewendet.
- Case Studies (Part-3, Section 6):
  - Die Ziele, die 'Problem Formulation', die Konzepte sowie die Ansätze zur Risiko-Charakterisierung wurden von mir entworfen und mit Kollegen der Ökotoxikologie von Bayer CropScience diskutiert.
  - Die verschiedenen technischen Tätigkeiten wurden von mir selbst und in teilweiser Unterstützung durch Kollegen durchgeführt (z.B. Vorbereitung von Geodaten durch J Wissing). Xplicit-Simulationen und Auswertungen wurden durch mich durchgeführt.
  - Die technische Anbindung von externen Modellen ('Associated Models') an das *Xplicit-Framework* und deren Konfiguration wurde durch S Bub unterstützt.

Hiermit erkläre ich an Eides statt, dass ich die Dissertation "*Xplicit – A Modelling Framework for Ecological Risk Characterisation at Landscape-scales in Regulatory Risk Assessment and Risk Management of Plant Protection Products*" selbstständig verfasst habe und keine anderen als die angegebenen Hilfsmittel verwendet habe. Die Anteile von Koautoren sind in dieser Erklärung wiedergegeben und in der Dissertation gekennzeichnet.

Die Dissertation wurde nicht für eine andere wissenschaftliche Prüfung eingereicht.

Leichlingen, Mai 2013