Simulating the impact of herbicide drift exposure on non-target terrestrial plant communities

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Univ. -Diss.
zur Erlangung des akademischen Grades
„doctor rerum naturalium“
(Dr. rer. nat.)
in der Wissenschaftsdisziplin „Ökologie“

Kumulativ eingereicht an der
Mathematisch-Naturwissenschaftlichen Fakultät
Institut für Biochemie und Biologie
der Universität Potsdam

Tag der Einreichung: 29. Januar 2019
Ort und Tag der Disputation: Potsdam, 30. April 2019

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https://doi.org/10.25932/publishup-42907
https://nbn-resolving.org/urn:nbn:de:kobv:517-opus4-429073

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I List of abbreviations

EC	European Commission
EFSA	European Food Safety Authority
ERx	Effect rate
IBC-grass	Individual-based community model for grasslands
NTTP	Non-target terrestrial plant
OECD	Organisation for Economic Co-operation and Development
PPP	Plant protection products
SPG	Specific protection goals
US EPA	United States Environmental Protection Agency

II Summary

In Europe, almost half of the terrestrial landscape is used for agriculture. Thus, semi-natural habitats such as field margins are substantial for maintaining diversity in intensively managed farmlands. However, plants located at field margins are threatened by agricultural practices such as the application of pesticides within the fields. Pesticides are chemicals developed to control for undesired species within agricultural fields to enhance yields. The use of pesticides implies, however, effects on non-target organisms within and outside of the agricultural fields. Non-target organisms are organisms not intended to be sprayed or controlled for. For example, plants occurring in field margins are not intended to be sprayed, however, can be impaired due to herbicide drift exposure. The authorization of plant protection products such as herbicides requires risk assessments to ensure that the application of the product has no unacceptable effects on the environment. For non-target terrestrial plants (NTTPs), the risk assessment is based on standardized greenhouse studies on plant individual level. To account for the protection of plant populations and communities under realistic field conditions, i.e. extrapolating from greenhouse studies to field conditions and from individual-level to community-level, assessment factors are applied. However, recent studies question the current risk assessment scheme to meet the specific protection goals for non-target terrestrial plants as suggested by the European Food Safety Authority (EFSA). There is a need to clarify the gaps of the current risk assessment and to include suitable higher tier options in the upcoming guidance document for non-target terrestrial plants.

In my thesis, I studied the impact of herbicide drift exposure on NTTP communities using a mechanistic modelling approach. I addressed main gaps and uncertainties of the current risk assessment and finally suggested this modelling approach as a novel higher tier option in future risk assessments. Specifically, I extended the plant community model IBC-grass (Individual-based community model for grasslands) to reflect herbicide impacts on plant individuals. In the first study, I compared model predictions of short-term herbicide impacts on artificial plant communities with empirical data. I demonstrated the capability of the model to realistically reflect herbicide impacts. In the second study, I addressed the research question whether or not reproductive endpoints need to be included in future risk assessments to protect plant populations and communities. I compared the consequences of theoretical herbicide impacts on different plant attributes for long-term plant population dynamics in the community context. I concluded that reproductive endpoints only need to be considered if the herbicide effect is assumed to be very high. The endpoints measured in the current vegetative vigour and seedling emergence studies had high impacts for the dynamic of plant populations and communities already at lower effect intensities. Finally, the third study analysed long-term impacts of herbicide application for three different plant communities. This study highlighted the suitability of the modelling approach to simulate different communities and thus detecting sensitive environmental conditions.

Overall, my thesis demonstrates the suitability of mechanistic modelling approaches to be used as higher tier options for risk assessments. Specifically, IBC-grass can incorporate available individual-level effect data of standardized greenhouse experiments to extrapolate to community-level under various environmental conditions. Thus, future risk assessments can be improved by detecting sensitive scenarios and including worst-case impacts on non-target plant communities.

III Allgemeinverständliche Zusammenfassung

Fast die Hälfte der gesamten Landfläche in Europa wird für landwirtschaftliche Zwecke genutzt. Daher sind halb-natürliche Gebiete, wie zum Beispiel Ackerränder, von besonderer Bedeutung für den Artenreichtum in intensiv genutzten Ackerlandschaften. Vor allem in den intensiv genutzten Äckern werden Chemikalien eingesetzt um die Erträge zu erhöhen. So werden zum Beispiel Pflanzenschutzmittel eingesetzt, um Unkräuter im Acker zu vernichten. Allerdings kann dieser Einsatz auch Auswirkungen auf sogenannte Nicht-Zielarten haben. Dies sind solche Arten oder Artindividuen, die z.B. innerhalb vom Acker nicht in Konkurrenz mit den darauf wachsenden Getreidesorten stehen oder sich nicht innerhalb vom Feld befinden aber dennoch den Pflanzenschutzmitteln ausgesetzt sind. Um den Artenreichtum in halb-natürlichen Gebieten zu schützen, ist es daher notwendig eine Risikoabschätzung durchzuführen bevor ein Pflanzenschutzmittel für den Verkauf und die Anwendung zugelassen wird. Für terrestrische Nicht-Zielpflanzen erfolgt eine solche Risikoabschätzung basierend auf standardisierten Gewächshausexperimenten, in denen die Effekte auf der Ebene von Einzelindividuen gemessen werden. Um das letztliche Risiko im Freiland für ganze Pflanzengemeinschaften abzuschätzen, werden sogenannte Unsicherheitsfaktoren hinzugenommen. Allerdings stellen neuere Studien in Frage, ob der derzeitige Ansatz ausreichend sicher ist. Dies gilt vor allem in Bezug auf die aktuellen speziellen Schutzziele, die den Fokus auf den Schutz von Pflanzengemeinschaften und Artenreichtum legen. Es ist daher zwingend notwendig die Wissenslücken der derzeitigen Risikoabschätzung zu schließen und Optionen zu weiteren Studien zu geben, die das Risiko vom Einsatz von Pflanzenschutzmitteln für Nicht-Zielpflanzen realistischer abschätzen können.

In meiner Dissertation nutze ich einen mechanistischen Modellierungsansatz um den Einfluss von Pflanzenschutzmitteln auf Nicht-Zielpflanzengemeinschaften zu untersuchen. Hierbei spreche ich die wesentlichen Wissenslücken und Unklarheiten der aktuellen Risikoabschätzung an und schlage zusammenfassend eine neue Option für eine realistischere Abschätzung des Risikos vor. Hierzu integriere ich den Einfluss von Herbiziden auf Einzelindividuen in das Pflanzengemeinschaftsmodell IBC-grass. In meiner ersten Studie vergleiche ich Modellvorhersagen von kurzzeitigen Herbizideffekten in künstlichen Artgemeinschaften mit experimentellen Daten. Mit der Studie zeige ich, dass das Modell den Einfluss von Herbiziden auf die Pflanzengemeinschaft realistisch vorhersagen kann. In

der zweiten Studie fokussiere ich mich auf die Frage, ob Effekte auf weitere Pflanzeneigenschaften, insbesondere Fortpflanzungseigenschaften, wie zum Beispiel die Samenproduktion, im Rahmen der standardisierten Gewächshausstudien gemessen werden sollten. Die Studie zeigt, dass die derzeitig gemessenen Pflanzeneigenschaften am meisten Einfluss auf die Dynamiken einer Pflanzengesellschaft haben und somit schon geringe Schädigungen dieser Eigenschaften auf Individuenebene Auswirkungen für die Gemeinschaft haben. Dahingegen führten nur sehr starke Effekte auf die Fortpflanzungseigenschaften zu einem Einfluss auf Gemeinschaftsebene. Mit der letzten Studie zeige ich, dass der Modellansatz dazu genutzt werden kann Auswirkungen für unterschiedliche Pflanzengemeinschaften darzustellen.

Zusammengefasst zeigen die Studien meiner Dissertation, dass mechanistische Modellierung eine geeignete Option für eine realistischere Risikoabschätzung ist. Auf Grund des besonderen Designs von IBC-grass können die durch derzeitige Gewächshausstudien zur Verfügung stehenden empirischen Daten in das Modell eingearbeitet werden und somit das Risiko auf Gemeinschaftsebene abgeschätzt werden. Mit Hilfe des Modells können mehrere Umweltbedingungen getestet werden und somit Extremszenarien abgedeckt werden. Meine Studien tragen dazu bei, zukünftige Risikoabschätzungen für Nicht-Zielpflanzen zu verbessern.

1 General introduction

1.1 Motivation

In the European Union, almost half of the total terrestrial area is used for agriculture. Crop production is one of the main agricultural practice with cropland covering 22.2% of the total terrestrial area (Eurostat, 2015). Starting in the 1940s, the development of chemical pesticides led to a frequent application on conventionally managed farms to increase the yields. The use of pesticides implies, however, effects on non-target organisms within and outside of the agricultural fields. In my thesis, I focus on the impact of herbicide application on non-target terrestrial plant communities adjacent to agricultural fields. In the following paragraphs, I give a short overview of pesticide exposure pathways to off-field areas. Subsequently, I focus especially on the adverse impacts of herbicide drift exposure for non-target terrestrial plants establishing the basis for risk assessments of terrestrial plants. I outline the current risk assessment procedure for these organisms including the underlying uncertainties. Next, I elaborate on the potential of ecological modelling approaches to address the arising research questions. Finally, I summarize the methodology and outline of my thesis, in which I aim to close the gap between the current risk assessment and the overarching goal to protect biodiversity in agricultural landscape.

1.1.1 Pesticide exposure to off-field areas

Applying pesticides on agricultural fields lead also to pesticide exposure in off-field areas mainly due to drift events. Pesticide drift is the movement of pesticide droplets away from the target area at the time of application (Olszyk et al., 2004). The two most important factors determining pesticide drift are the application method and the weather. Boom sprayers are frequently used to apply liquid pesticide formulations. The design of these sprayers is quite diverse and each single design aspect can influence the probability of drift. For example, with decreasing droplet sizes the risk increases that these small droplets move into unintended areas. But also the pressure, the spraying height and the driving speed influence the drift potential (Wang and Rautmann, 2008). Besides the application method, also weather conditions play an important role for the drift potential, especially wind speed and direction (Wang and Rautmann, 2008). Higher wind speed and downwind direction can lead to a higher drift potential. In extensive drift experiments Ganzelmeier et al. (1995) and Rautmann et al. (2001) measured drift exposure in non-target areas in order to calculate drift rates that can be used to predict the potential for non-target areas to have an unintended exposure to pesticides. Ganzelmeier et al. (1995) did 119 drift measurements in various agricultural fields (crop fields (16 trails), grapevine (21 trials), fruit crops (61 trials) and hops (21 trials)). For field crops, 0.26 – 3.51 % of the application rate were found in 1m distance and still in 3m distance from the edge of the field, almost 1% of the application rate were detected. Based on these trials and assuming an application according to Good Agricultural Practice (wind speed is lower than 5 m/s and the temperature is lower than 25°C), basic drift values can be calculated (considering the 90th percentile of the individual trials). For field crops, a drift of 2.77% is considered in 1m distance to the edge of the field; decreasing to 0.29 % in 10m distance. With increasing number of applications, the basic drift values are also decreasing (Rautmann et al., 2001). As pesticides are specifically designed to control undesired organisms in the field, the drift into adjacent areas can lead to undesired effects in non-target areas.

1.1.2 Consequences for non-target species, populations and communities

Among the different pesticides, herbicides have the highest impacts on non-target terrestrial plants as they are specifically designed to control plant species competing with crops and thus leading to a decrease in yields; so called weed species. However, undesired within agricultural fields, these plant species drive the plant diversity in field margins and thus in semi-natural landscapes. Worldwide herbicides are even the most frequently applied pesticides (Sanchez-Bayo et al., 2012) and are one of the main drivers for plant diversity loss in non-target areas (Andreasen and Streibig, 2011). Marrs et al. (1989) detected lethal effects of three herbicides mainly in 1-3m distance to the edge of the field. However, for some plant species, like *Prunella vulgaris* or *Lynchnis flos-cuculi*, only at 5 m distance no lethal effects were observed. Furthermore, herbicide exposure also shifts plant community composition. In a community field experiment consisting of 4 different plant species, Pfleeger et al. (2014) detected a community shift at 10% of the full application rate of Glyphosate and at 3.7% of the full application rate of aminopyralid. In a microcosm experiment, Dalton and Boutin (2010) also observed changes in community structure.

In addition to the direct impacts on plants and plant communities, a shift in the community structure can also have undesirable impacts on other organisms in the ecosystem. Field boundaries, semi-natural vegetated habitat strips consisting of herbaceous plants, hedges or trees, have a variety of beneficial ecological functions at a local, but also at a landscape scale. Locally, field boundaries can serve as shelter for prey species to hide from predators within the agricultural landscape (Buckelew et al., 2000; Denys and Tscharntke, 2002), feeding habitat (Moreby and Southway, 1999) or breeding habitat and thus promoting wildlife in agricultural areas (Lazzerini et al., 2007; Morrison et al., 2017; Rodríguez-Pastor et al., 2016). Species rich field margins support populations of pollinator species, which are crucial for the productivity within the agricultural field (Free, 1993). On a landscape scale, field boundaries can be an important migration pathway within the agricultural landscape and thus play a major role for meta-community dynamics or movement ecology. The relevance of connectivity between habitat patches is increasing as field sizes increase. For example, negative impacts of agricultural practices on plant populations can be compensated by sufficient landscape structure and connectivity (Tscharntke et al., 2005). To conclude, a shift in the structure and composition of field margins can lead to indirect effects on invertebrates and vertebrates. Thus, the regulation of the authorization and the use of herbicides in agriculture to avoid harmful effects on non-target terrestrial plants is not only important for the plants themselves, but also for the whole ecosystem functioning.

1.1.3 Current regulations – the need for improvement

The directive 1107/2009 regulates the authorization of pesticides in the European Union (EU). It states that an active substance "shall only be approved if the risk assessment demonstrates risks to be acceptable" (EC, 2009). For several organisms, the European Food Safety Authority (EFSA) published guidance documents, which should advice the regulators in risk assessments according to the EU directive (e.g. aquatic organisms (EFSA PPR Panel, 2013) or birds and mammals (EFSA PPR Panel, 2009)). However, for non-target terrestrial plants the EFSA guidance document is still under development and so far, only a scientific opinion was published, which highlights the importance of terrestrial plants for ecosystem services and defines specific protection goals on population and community level (EFSA PPR Panel, 2010, 2014a). Currently the risk assessment for non-target terrestrial plants is covered by the OECD guidance documents 208 and 227 (OECD 2006a, 2006b), which define structured and standardized greenhouse experiments. In the seedling emergence study (OECD, 2006b), the seedling emergence and seedling growth are assessed whereas the vegetative vigour study (OECD, 2006a) covers the effects on young plants and assesses the impacts on plant growth and survival; assessments of visible detrimental effects on different parts of the plants are included in both studies. As these experiments measure the impacts on plant individual-level only on selected plant species and in the greenhouse, assessment factors are applied to account for uncertainties and to extrapolate the effects to population level in the field. Nevertheless, clear protection goals are still missing for non-target terrestrial plants and it is unclear whether the current approach can be protective for addressing the specific protection goals mentioned in the EFSA scientific opinion (EFSA PPR Panel, 2010).

Three main drawbacks of the current approach are often addressed in recent studies. First, the uncertainty of the assessment endpoints is questioned by several researchers, who claim that reproductive endpoints need to be included (Boutin et al., 2014; Carpenter et al., 2013; Riemens et al., 2008, 2009). Currently, only the impact on plant dry weight, emergence and survival are measured assuming that these are the most sensitive endpoints. However, Riemens et al. (2009) showed that for 3 out of 6 tested plant species the reproductive endpoints had lower sensitivities than the vegetative vigour endpoints. Carpenter et al. (2013) measured long-term effects on reproduction and found significant impacts in 3 out of 5 tested plant species. Impacts on reproduction are especially important for annual plants, for which seed production is an important driver maintaining a population.

Furthermore, the representativeness of the test species is questioned (Boutin et al., 2004; Boutin and Rogers, 2000; Strandberg et al., 2012). 6 to 10 plant species are tested in a standard greenhouse experiments. The test species need to have a high germination probability and need to be grown in greenhouses, which results in few weed species but many crop species being tested. Thus, it is questionable whether high sensitive plants would be protected by the current risk assessment. An assessment factor of 10 is currently applied to cover for this uncertainty. Christl et al. (2015) conducted a literature review collecting data of ecotoxicological studies comparing the sensitivity of weed and crop species. This study showed that an assessment factor of 10 was protective for many weed and crop species.

Finally, the current risk assessment measures the impact on plant individual-level. This is not in accordance with the specific protection goals which are on plant population or even community level to cover for impacts on diversity (EFSA PPR Panel, 2014a). To extrapolate from individual-level effects to community-level, the impact of inter- and intraspecific competition and the variation in susceptibility needs to be accounted for. Field experiments on community level can be used to estimate community-level impacts in future risk assessments (de Snoo and van der Poll, 1999; Kleijn and Snoeijing, 1997; Marrs and Frost, 1997; Schmitz et al., 2014; Strandberg et al., 2012). However, there are major limitations of regular field testing: the standardization, representativeness and the limitation of spatial resources. Natural variability is high in field studies. Thus, a higher amount of repetitions is necessary to detect differences between treatments. As the environmental conditions within a study cannot be controlled, field studies cannot be repeated and a comparison between different field studies is impossible, even if the experimental design is similar. Furthermore, disentangling the herbicide impact from effects due to other agricultural practices or environmental conditions is not feasible as a full factorial design is restricted due to spatial and financial resources. Another drawback of field tests is the representativeness of a community for different countries or even areas within a country making it nearly impossible to find a suitable reference community.

In summary, the two main uncertainties in the current risk assessment for non-target terrestrial plants are the protectiveness of the currently measured assessment endpoints for the stability of plant populations and the extrapolation of individual-level effects to a plant community level including the extrapolation from test species to non-crops species in field boundaries. This highlights the importance of revising the current risk assessment approach for non-target terrestrial plants in the EU according to the scientific state of the art and the specific protection goals for non-target terrestrial plants (EFSA PPR Panel, 2010, 2014a).

1.1.4 Ecological simulation models as extrapolation tool

The research field of ecological modelling emerged from the field of theoretical ecology which breaks down drivers and complex systems or dynamics to basic underlying rules and processes (e.g. Lotka-Volterra predator-prey interactions (Berryman, 1992)). Ecological models aim to understand and identify main drivers of complex ecological systems and their dynamics. Sophisticated models are able to reflect dynamics of complex systems and to make general conclusions about system behavior. There is a broad range of different modelling approaches, from mathematical models to mechanistic models. In ecology, models are well accepted tools to predict future development or behaviour of populations or systems (e.g. population viability analyses (Brook et al., 2000) or climate change models (Meehl et al., 2007)) or to extrapolate to higher organizational levels (e.g. from individual to population level in population viability analyses).

In ecological risk assessment, the spatial and temporal limitations as well as the labour and financial costs of experimental field studies can be overcome by such ecological simulation models, whose limits are mainly defined by computational resources. Using an ecological model, a range of different environmental scenarios can be tested using a full factorial design. The variability within a model resulting from stochastic processes can be covered by increasing the number of repetitions. In contrast to field studies, the number of repetitions can be increased without exceeding the spatial limitations. EFSA acknowledged that ecological models can have the potential to close the gaps of current risk assessment for non-target terrestrial plants (EFSA PPR Panel, 2014a). They mention that ecological models can be used to identify vulnerable ecological scenarios, which need to be tested during the environmental risk assessment, and to extrapolate individual-level effects to populations and communities, but also to extrapolate from short-term to long-term effects in space and time. The MODELINK workshop summarized how ecological models can be integrated in future risk assessments (Hommen et al., 2016). For six case studies covering a wide range of different groups of organisms the researchers presented how available data from standard ecotoxicological tests can be linked to protection goals.

In general, to be considered as a tool for risk assessments, a model needs to be compared to real data, proving that the simplified model can actually represent real world conditions and make valid predictions (Grimm and Martin, 2013). In addition, a thorough sensitivity analyses of the model parameters, especially those parameters not based on empirical data, is needed to show the robustness of the model. Guidance documents help researchers to log the development of their model and facilitate the communication between model developers and users, e.g. regulators, by presenting the applicability and capabilities of the model (e.g. EFSA PPR Panel, 2014a; Grimm et al., 2014).

1.2 Objectives and methodology

The overarching goal of my thesis is to improve the understanding of herbicide exposure impacts on non-target terrestrial plant communities. With my thesis, I aim to close the gap of the current risk assessment approach for non-target terrestrial plants and the specific protection goals (EFSA PPR Panel, 2014a). With that I want to propose a novel tool for future risk assessments and for supporting the decision making of risk assessors and risk regulators. In particular, I want to address three specific research questions, namely: (i) can the plant community model realistically predict herbicide induced effects on plant biomass in community context? (ii) are the plant endpoints currently used protective for plant populations? and (iii) will different plant communities behave differently under herbicide exposure?

1.2.1 The plant community model IBC-grass

I use a modelling approach to address the research questions mentioned above. The plant community model IBC-grass (Individual-Based Community model for grasslands) is a well-established plant community model which simulates plant community dynamics on a local scale. It was first developed as a theoretical study by May et al. (2009). Weiß et al.

(2014) extended the theoretical model and studied the effect of different grazing intensities of grasslands in the Uckermark, Germany. The researchers compared patterns in the model with empirical data and were able to reflect similar biomass and species richness pattern under low, medium and high grazing intensities. Körner et al. (2014) and Pfestorf et al. (2016) used the model to analyse effects of belowground herbivores.

MAIN PRINCIPLES OF IBC-GRASS

The model uses an individual-based and spatially explicit approach. Individual plants are located on a grid representing a small-scale plot in the landscape (Fig. 1.1). The model differentiates between the aboveground and the belowground compartment. The plant individuals interact with each other based on specific principles. Thus, community dynamics emerge from individual plant behaviour.

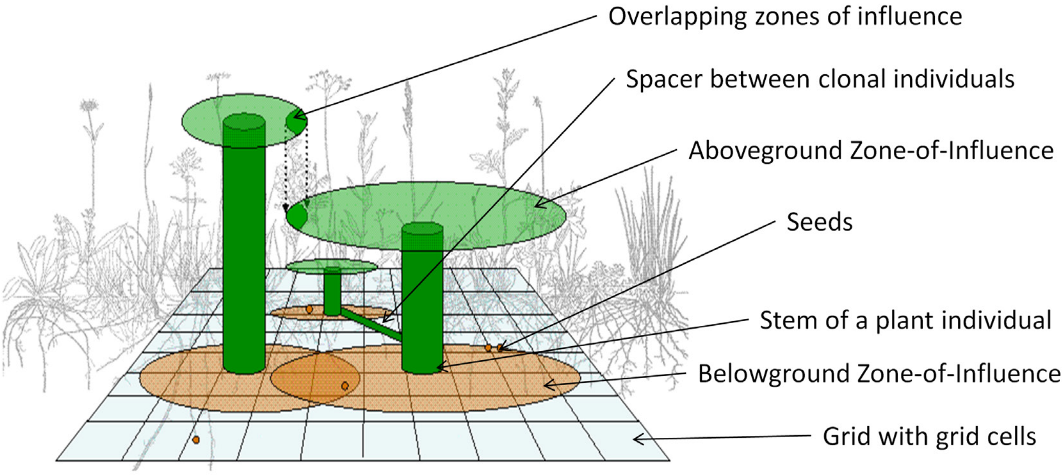

Figure 1.1: Graphical scheme of the IBC-grass model. Graphic adapted from Weiß (2017).

In order to allow for general conclusions, the model applies a trait-based approach. Plant traits, known to be important drivers for plant-plant interactions, are selected in order to group plant species into plant functional types (PFTs). It is known that a trait-based approach can be used to link plant diversity to ecosystem functions or environmental stressors (De Lange et al., 2009; Díaz and Cabido, 2001). The trait characteristics determine the competitive ability of plants and their behavior (growth and mortality). This approach is in line with the EFSA opinion, stating the advantages of using trait-based approach for the description of communities or for facilitating the comparison of different plant communities (EFSA PPR Panel, 2014a).

To account for competition between plant individuals, the Zone of Influence approach (ZOI) is used. It calculates a circular area (the ZOI area) around the stem of each individual in which it takes up resources. Thereby, model distinguishes between the belowground and the aboveground compartment. In overlapping ZOIs, plants compete for resources and thus for space. The competitive ability of plant individuals is determined by the specific trait characteristics. In the belowground compartment the resources are distributed symmetrically, whereas aboveground taller plants allocate a higher amount of resources to reflect shading effects.

Simulating specifically plant individuals, individual-level effects measured in the current standardized greenhouse experiments can be transferred to plant individuals in the simulated plant community. Furthermore, several processes potentially influenced by herbicide exposure can be addressed in the model: a reduction of plant biomass, a reduction of seedling biomass, an increase of plant mortality, a decrease in the establishment of seedlings ,a reduction in seed number and an increase in seed sterility (seeds are not able to germinate).

1.2.2 Outline

I address the research questions in three chapters, which I outline in the following. Each chapter can be read independently from each other.

In the second chapter[1], I use the study of Reuter and Siemoneit-Gast (2007) to compare model predictions to empirical data. Reuter and Siemoneit-Gast conducted a semi-field experiment for two herbicides, a selective-herbicide and a broad spectrum herbicide. They measured effects on the biomass of 6 different weed species grown in monocultures as well as in artificial communities. To clearly differentiate between model parametrisation and true model predictions, I only use the monoculture data to parameterize the IBC-grass model and to calculate individual-level effects using dose-response data. Afterwards, I compare the predicted effects in the artificial communities to the empirically measured effects by Reuter and Siemoneit-Gast (2007). The model shows similar pattern as observed in the empirical data and thus, is able to realistically reflect herbicide induced effects on plant biomass. Although this is only a short-term study, it increases the credibility of the model IBC-grass to be used for predicting long-term herbicide impacts on plant communities.

In the third chapter[2], I aim to give insights into the influence of the different plant attributes potentially affected by herbicides and the resulting impact on plant populations

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[1] published as: Reeg J, Heine S, Mihan C, McGee S, Preuss TG, Jeltsch F. 2018. Simulation of herbicide impacts on a plant community: comparing model predictions of the plant community model IBC-grass to empirical data. Environ Sci Eur 30:44. DOI: 10.1186/s12302-018-0174-9

[2] published as: Reeg J, Heine S, Mihan C, Preuss TG, McGee S, Jeltsch F. 2018. Potential impact of effects on reproductive attributes induced by herbicides on a plant community. Environ Toxicol Chem. 37(6):1707-1722. DOI: 10.1002/etc.4122

in community context. To address this question, I select vegetative as well as reproductive plant attributes, which are assumed to be affected by herbicides: biomass, mortality, establishment, seed number and seed sterility and, furthermore, included effects passed on to the next generation (F1 generation). I vary the effect intensity on each of the attributes from 10- 90% in 10% intervals. To account for different modes of action of the theoretical herbicide, either all, only competitive, only less-competitive, only monocotyledonous or only dicotyledonous PFTs are affected. In this study, I analyse which affected plant attributes has higher impacts on the plant community dynamics and which effect intensities actually result in significant impacts on population and community level. An herbicide-induced increase of plant mortality and seed sterility has the highest impacts on the plant community, especially if the herbicide was selective for one specific group. The other reproductive attributes, namely seed number and establishment, have only an impact on plant community level, when the effect is very strong. When herbicide impacts are passed on to the next generation, the long-term impact on population and community level strongly increase. This sensitivity analysis of the potentially affected plant attributes shows that the most sensitive attribute for the protection of plant populations and communities – plant mortality – is already covered in the current risk assessment for non-target terrestrial plants. Effects on plant biomass are compensated over the year. Only a strong effect intensity on seed number results in significant effects on plant populations. Though producing a lower amount of seeds, plants can still emerge from the seed bank. However, if a herbicide is known or suspected to have a strong impact on the reproduction of plants, it should be considered in risk assessments. This study highlights that the model IBC-grass can be a suitable tool to estimate potential risks and help to decide whether the impact on seed productions needs to be accessed by empirical studies.

The fourth chapter[3] focuses on direct and indirect impacts of herbicides on plant populations in community context of three different plant communities. In this study, I investigated whether plant communities, which differ in their species composition, the nutrient level and disturbance regimes, show different sensitivities towards a potential herbicide exposure. I choose three plant communities typical for Germany. The first community consists of plant species occurring in field boundaries (based on a literature review of Kolja Bergholz, University of Potsdam (unpublished)). This community has high nutrient levels and few disturbances by trampling and grazing. It is mowed once a year. The other two communities represent grasslands. *Arrhenatheretalia* represents a nutrient rich grassland

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[3] published as: Reeg J, Schad T Preuss TG, Solga A, Körner K, Mihan C, Jeltsch F. 2017. Modelling direct and indirect effects of herbicides on non-target grassland communities. Ecological Modelling. 348: 44-55. DOI: 10.1016/j.ecolmodel.2017.01.010

with few disturbances by grazing and trampling. It is mowed three times a year. *Calthion* represents a nutrient poor grassland with lower disturbances by grazing and cutting and only one mowing event per year. In this study, I use the herbicide exposure model Xplicit to calculate first the exposure rate in several distances to the agricultural field, but also to calculate species effect distributions based on the previously calculated exposure rates. In this way, I am able to predict herbicide effects in varying distances to the field. This study shows that the three plant communities differ in their susceptibility. Especially the *Calthion* community shows strong impacts in direct neighbourhood of the arable field as the plant species occurring in this community are not adapted to disturbances. Thus I focus on this community in the subsequent analyses of population-level impacts. On population level, one can clearly see also indirect effects of the herbicides. Some PFTs benefit from the herbicide induced disturbance and can even increase in their population size and some PFTs show stronger negative impacts than others. These effect patterns can be explained by the trait characteristics of the specific PFTs. This study highlights that different plant communities can be reflected in IBC-grass. Thus, reference communities can be developed for future risk assessments as surrogates for typical communities in European countries.

Finally, a general discussion follows the first three chapters. First, I discuss the overall achievements of the three studies presented with regard to the current risk assessment. I suggest future directions of how the model can be coupled with standard greenhouse experiments in order to be a higher tier option in future risk assessments. In addition, I discuss how other legislative directives can be used to protect non-target terrestrial plants such as mitigation measures or the good agricultural practice. I close my discussion with an overall conclusion of my thesis and a future application in risk assessments.

The thesis is in a cumulative form. The chapters 2-4 are co-authored and published in peer-reviewed journals. The contents are identical to the published articles in the scientific journals and thus are written in first-person plural. I am the first author of these publications and thus, I have performed the main work in the studies. I implemented the model extensions, parameterized the model, analysed the data and wrote the manuscripts. I discussed the study concepts and results with my coauthers. In addition, my coauthors supported me in writing the manuscripts. The references can be found altogether at the end of the thesis.

2 Simulation of herbicide impacts on a plant community: comparing model predictions of the plant community model IBC-grass to empirical data[1]

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[1] published as: Reeg J, Heine S, Mihan C, McGee S, Preuss TG, Jeltsch F. 2018. Simulation of herbicide impacts on a plant community: comparing model predictions of the plant community model IBC-grass to empirical data. Environ Sci Eur 30:44. DOI: 10.1186/s12302-018-0174-9

2.1 Abstract

Semi-natural plant communities such as field boundaries play an important ecological role in agricultural landscapes, e.g., provision of refuge for plant and other species, food web support or habitat connectivity. To prevent undesired effects of herbicide applications on these communities and their structure, the registration and application are regulated by risk assessment schemes in many industrialized countries. Standardized individual-level greenhouse experiments are conducted on a selection of crop and wild plant species to characterize the effects of herbicide loads potentially reaching off-field areas on non-target plants. Uncertainties regarding the protectiveness of such approaches to risk assessment might be addressed by assessment factors that are often under discussion. As an alternative approach, plant community models can be used to predict potential effects on plant communities of interest based on extrapolation of the individual-level effects measured in the standardized greenhouse experiments. In this study, we analysed the reliability and adequacy of the plant community model IBC-grass (individual-based plant community model for grasslands) by comparing model predictions with empirically measured effects at the plant community level.

We showed that the effects predicted by the model IBC-grass were in accordance with the empirical data. Based on the species-specific dose responses (calculated from empirical effects in monocultures measured 4 weeks after application), the model was able to realistically predict short-term herbicide impacts on communities when compared to empirical data.

The results presented in this study demonstrate an approach how the current standard greenhouse experiments—measuring herbicide impacts on individual-level—can be coupled with the model IBC-grass to estimate effects on plant community level. In this way, it can be used as a tool in ecological risk assessment.

2.2 Background

With agricultural landscape covering almost half of the European land area, it is reasonable that environmental impact of agricultural practices is evaluated. Of particular interest are the potential impacts of pesticide applications, which regulatory authorities around the world are required to evaluate and make regulatory decisions on the acceptability of potential risks to the environment. Pesticides are designed to control pests, including competing weed species in agricultural fields, thereby increasing the yields. However, small amounts of these pesticides may reach adjacent off-field areas, the so-called non-target areas (de Jong et al., 2008; EFSA PPR Panel, 2014a). To prevent undesired effects of an herbicide application, the registration and application are regulated by risk assessment schemes in many industrialized countries (EPPO, 2003). To characterize the effects of herbicide loads potentially reaching off-field areas on plants, standardized individual-level greenhouse experiments are conducted on a selection of crop and wild plant species (OECD, 2006a, 2006b; USEPA, 2012a, 2012b).

To account for uncertainties associated with extrapolating from testing plant individuals in the greenhouse to plant communities in the field, an assessment factor may be applied. However, the appropriateness of the assessment factor can be debated as currently there is no reference tier that would allow for calibration. Extending the standard ecotoxicological tests for non-target terrestrial plants under worst-case greenhouse conditions to more realistic field conditions or community level is not feasible. Not only reproducibility is a major constraint, but there is also the question of representativeness of higher tier studies for different landscapes under different climatic conditions. Additional data are needed to reduce uncertainty associated with predicting the potential long-term impacts on non-target terrestrial plant communities from short-term individual-level greenhouse studies.

Several researchers investigated specific uncertainties associated with the current standard test guidelines (OECD, 2006a, 2006b). Many of these focus on comparing individual-level standard experiments conducted in greenhouses versus in the field. They assess the level of protection when using greenhouse experiments to predict expected effects under field conditions (Fletscher et al., 1996; Pfleeger et al., 2012; Riemens et al., 2009). Although it was generally shown that the effects on single species observed in the greenhouse are more pronounced than under field conditions and, therefore, lead to a conservative risk assessment, these experiments cannot illustrate the influence of competition between individuals of different plant species. Only few studies focused on artificial communities to account for these processes (Pfleeger et al., 2014; Reuter and Siemoneit-Gast, 2007). Both studies are based on a small species pool (4 and 6 plant species) and thus do not represent the diversity and composition of plant communities observed in environments that may receive off-site herbicide exposure. Real field studies testing the impact of in-field herbicide application on plant communities adjacent to the arable field are rare (e.g., Strandberg et al., 2012; Schmitz et al., 2014). Thus, general conclusions of the herbicide impact on plant communities under various environmental conditions cannot be made.

In nature conservation, modelling approaches are frequently used to overcome the limits of experimental studies and make general predictions on long-term impacts of, for example, climate change or grazing intensity (Rastetter et al., 2003). Cousins et al. (2003) highlight that landscape models are a useful method to increase the understanding of mechanisms affecting grassland communities due to land use change. Such ecological models have the advantage to cover a variety of different environmental scenarios and therewith a wider range of potential impacts than empirical studies, which are often limited in space and time. These studies highlight that modelling approaches can be valuable tools to address uncertainties in the current risk assessment scheme by analysing potential long-term impacts on community level.

In this study, we analysed the reliability and adequacy of the plant community model IBC-grass by comparing model predicted and experimentally measured effects at the plant community level. IBC-grass is an individual-based and spatially explicit plant community model; thus, individual-level effects from standard greenhouse studies can be integrated and competition between plant individuals is accounted for. We adjusted the model to the settings in the empirical study of Reuter and Siemoneit-Gast (2007); using one part of the data set for calibration (control data and dose–responses after herbicide application of the monocultures on individual plant basis). We evaluated if the calibrated model is able to predict similar plant community-level effects as observed in the empirical data (second part of the data set) and analysed to which degree the model is able to reproduce realistic effects by calculating model adequacy and reliability as a measure for the model fit (Scholten and Van der Tol, 1994).

2.3 Methods

2.3.1 Short summary of the experimental study design

Based on the results of a pre-study in which the researchers tested the germination rate and handling of plants, Reuter and Siemoneit-Gast (2007) tested their proposed higher tier study design on 6 wild plant species: *Bromus erectus*, *Cynosurus cristatus*, *Galium mollugo*, *Leontodon hispidus*, *Silene nutans* and *Trifolium pratense*. Plant individuals were transplanted into monocultures and communities after reaching the growth stage BBCH 12–14. In the monoculture setup, 4 individuals of the same plant species were transplanted into a pot with a diameter of 7 cm. In the artificial communities, 8 individuals per plant species were transplanted randomly in square pots of 17 × 17 cm. The distance between each individual was 2.5 × 2.6 cm. The remaining space in the center of each pot was planted with an individual of a randomly chosen species. Monoculture setup included 4 repetitions for each of the 3 assessment dates (i.e., overall 12 pots per treatment); community setup included 3 repetitions per assessment date (i.e., overall 9 pots per treatment). The researchers used the experimental setup to investigate two different herbicides: a broad spectrum herbicide, RoundUp® (active ingredient glyphosate), and a selective herbicide, Monitor® (active ingredient sulfosulfuron). Five different test item rates (3, 5, 9, 15, 25% of the maximal application rate of 3 L/ha RoundUp® and 5, 9, 17, 31 and 55% of the maximal application rate of 25 g/ha of Monitor®) and a control were tested per herbicide. In the EU, the current off-field risk assessment approach assumes 2.77% of an application in field crops might drift of the target application site. This drift rate accounts for normal farming practice and machine operation and assumes wind direction into the off-field area. The lowest rates tested were in the same range (RoundUp®) or higher (Monitor®) than the rates that would be used in a baseline EU risk assessment to assess the potential risk from exposure to off-field areas in 1 m distance. Fresh shoot weight and phytotoxicity were measured every 2 weeks over 6 weeks; however, only results for shoot weight could be compared to the model predictions, as the model is designed and developed to simulate biomass and not phytotoxicity. In addition, the assessment of phytotoxicity is a very subjective measure and a conversion of symptoms into effects on biomass would not be feasible. For more details, see Reuter and Siemoneit-Gast (2007).

2.3.2 IBC-grass

The spatially explicit and individual-based plant community model IBC-grass was originally designed to test the response of plant communities to different disturbances such as grazing (May et al., 2009; Weiß et al., 2014; Reeg et al., 2017; Reeg et al., 2018a). The main processes such as inter- and intraspecific competition for space and resources, growth, mortality and disturbances like grazing, trampling, mowing and herbicide impact are accounted for. A detailed description of the IBC-grass version on which this study is based on can be found in the appendix of Reeg et al. (2017). It follows the ODD (overview, design concept and details) protocol (Grimm et al., 2010). Here, we will give only a short overview of the main aspects and focus on the modifications and adaptions we integrated in the model to reconstruct the exposure scenario from the study of Reuter and Siemoneit-Gast (2007) to evaluate the precision of the model predictions.

General description of the main principles and processes

Plant functional type approach

To allow for general conclusions, plant species are classified into plant functional types (PFTs) according to important trait characteristics. This functional type approach is widely used in community ecology to explain dynamics in ecosystems (Gross et al., 2017). Experimental studies proved that the response of plant species with similar trait characteristics to environmental conditions and disturbances is comparable. Six different traits and trait syndromes (i.e., a group of traits representing general trade-offs) are distinguished in IBC-grass: growth form, plant size (correlated with seed mass, and dispersal traits), resource response (correlation of competitive ability and stress-tolerance), grazing response and clonality. Plant species of the species pool of interest are classified into PFTs based on trait information in the databases BiolFlor, LEDA and cloPla3 (Kleyer et al., 2008; Klimešová and de Bello, 2009; Klotz et al., 2002).

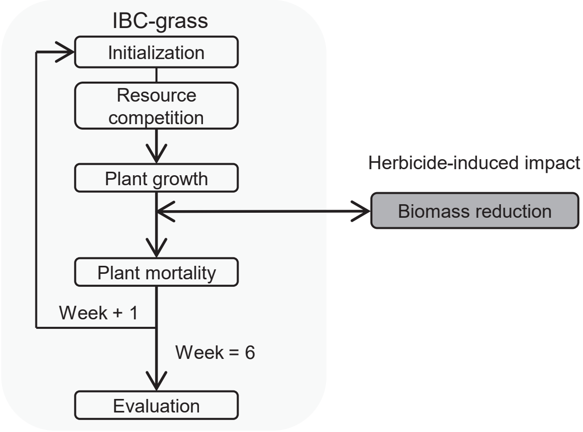

Figure 2.1: Flowchart of the processes in the current version of IBC-grass. Several processes such as seed production, seed dispersal and biotic disturbances such as grazing are omitted in this version due to the short time scale of the experiments.

Zone of influence approach

Intra- and interspecific competition is accounted for in the aboveground and in the belowground compartment. Plant individuals acquire resources within a circular area around the stem—their zone of influence (ZOI). For the belowground compartment, the size of the ZOI is determined only by the root biomass. It is assumed that plants have similar root geometries. Aboveground, the ZOI of a plant is determined by the shoot biomass and shoot geometry accounting for taller plants and shading effects. In overlapping ZOI areas, plant individuals compete for resources. Belowground, competition is simulated size-symmetrically. Thus, the distribution of resources in overlapping areas only depends on the competitive ability of the PFTs (resource response traits). Aboveground, resource competition is partially size-asymmetrically accounting for shading effects of taller plants. For both compartments, intraspecific competition is stronger than interspecific competition.

General processes

Figure 2.1 gives a general overview of all processes accounted for in this current IBC-grass version. Several processes important for long-term community dynamics are excluded in this version due to the short-term time scale of 6 weeks in the experimental study. In the following, the main processes applied in this version of IBC-grass are explained. For more details, see the appendix of Reeg et al. (2017).

plant growth and mortality. As mentioned before, plants acquire resources within their ZOI and compete for resources in overlapping areas. The acquired resources are allocated to the roots and shoot, and converted into biomass based on a constant conversion rate, the current shoot (root) mass, the trait characteristics of the shoot (root), the growth form, the maximal resource utilization and the maximal plant mass. In the absence of competition, the growth function results in a sigmoid growth (see also in Berger et al., 2008; DeAngelis and Mooji, 2005). Since the experimental study traced plant biomass over a time frame of 6 weeks and the researchers did not observe any mortality, we excluded mortality in this version. However, it is an important process for long-term community dynamic. A detailed description of how mortality is modelled in IBC-grass can be found in the ODD protocol of Reeg et al. (2017).

seed dispersal, germination and establishment. These processes are important for community dynamics. However, since the time frame of the experimental study is limited to 6 weeks, these processes have no impact on the results. The young plant individuals are not yet producing seeds. In this specific study, we used a 100% germination and establishment rate for the plant individuals (see *Spatial set up* in *Model Preparation*). A detailed description of the implemented process can be found in the ODD protocol in the appendix of Reeg et al. (2017).

biotic disturbances In this version, we excluded all biotic disturbances, such as grazing, tramping and cutting. We only integrated the herbicide impact.

abiotic factors and temporal dimensions IBC-grass distinguishes aboveground and belowground resource availability. For both compartments, resources are distributed homogeneously in space and time. One time step in the model represents 1 week.

2.3.3 Model preparation

SPATIAL SETUP

We adjusted the spatial initial setup in the model to mimic the experimental setup (Table 2.1). The grid size of the model was set to 7 × 7 grid cells, representing a 7 × 7 cm^2 pot, for the monocultures, and 20 × 20 grid cells, representing a 20 × 20 cm^2 pot for the artificial communities. In the monoculture setup, we distributed 4 seeds of the same PFT on the grid. Seeds had a distance of 2 grid cells to one another. The 4 seeds germinated with a probability of 100%, resulting in 4 young plant individuals located in the grid. In the model, herbicide treatment started according to the time of transplanting in the experiments (Table 2.2). The spatial setup in the modelled communities was adjusted according to that in the experiments: for each species, 6 plant individuals were initialized randomly in the grid with a distance of 2 grid cells to each other. The grid cell located in the middle was initialized with a randomly chosen plant individual. As mentioned before, initial plant biomasses in the communities were based on the biomasses in the monoculture set up (in the model) at the time of reaching the BBCH 12–14 in the experiment (Table 2.2).

Table 2.1: Overview of the experimental setup compared to the model set up.
Since IBC-grass simulates only rectangular plots, it is not able to represent a circular pot of 7 cm diameters. As the model assumes that plant individuals cannot grow beyond the plot size, we chose to use a greater area (7 × 7 cm) rather than a smaller one (6 × 6 cm) to account for potential shoot growth beyond the pot size. There was no information about the distance between plant individuals within the monoculture setup of the experiment. Therefore, we decided to use a similar distance as in the community set up. This also results in an even distribution of individuals within the plot

	IBC-grass	Experimental study
Monoculture		
Plot size	7 x 7 cm^2	ø 7 cm
Nb. of individuals	4	4
Distance between individuals	2 cm (2 grid cells	No information
Community		
Plot size	20 x 20 cm^2	17 x 17 cm^2
Nb. of individuals	49	49
Distance between individuals	2 cm (2 grid cells)	2.5 x 2.6 cm^2

Table 2.2: Compared biomasses in the model and the experiment.
Due to the different germination times and growth rates, the age of the plant individuals when being transplanted in the experiments differs between species. e.g., B. erectus was transplanted at the age of 2 weeks. In this case, herbicide treatment in the simulated monoculture started 2 weeks after germination and initial biomasses in the community setup are based on these biomasses (biomasses 2 weeks after germination in the simulated monocultures). In the analyses of B. erectus in the monoculture, the simulated biomasses of plants 4, 6 and 8 weeks after germination are equivalent to the biomass measurements of week 2, 4 and 6 in the experiments.

Species	Week >75% emergence	Week BBCH 12-14	Age at potting in the experiment (‚week 0‘ in the modeled monocultures)
B. erectus	2	4	2
C. cristatus[a]	2	2	0
G. mollugo	2	3	1
L. hispidus	2	3	1
S. nutans	3	4	1
T. pratense	1	3	2

[a] BBCH12-14 is reached between 2 and 3 weeks

MODEL CALIBRATION

In the following section, we will describe the process of calibrating the model against the monoculture control and effect data. All model parameters and settings are summarized in 7.1.1.

RESOURCE LEVELS IN IBC-GRASS

As the model is not considering concrete resources such as nutrients, soil moisture or light, but groups all kinds of resources into overall resource units, we cannot specify resources in a numerical way, e.g., % $CaCO_3$. To find the resource unit levels for the aboveground and belowground compartment, which result in similar growth patterns as in the experiments, we used Latin Hypercube Sampling (LHS; Iman, 1999). Therewith, we uniformly covered the whole potential sampling space. We selected these resource levels, for which the simulated shoot masses fell within the empirically measured shoot masses. We used only the monoculture control data for this calibration step, in order to have an independent validation on the community growth. Additionally, although Reuter and Siemoneit-Gast (2007) used different soils for the two herbicides and conducted the studies in spring and in summer, we combined the shoot masses for all control monocultures to have a higher sampling size (N = 8). This process is based on the pattern-oriented modelling approach (Grimm et al., 2005; Wiegand et al., 2003), which aims at comparing the patterns predicted by a model with patterns observed in the nature, e.g., the temporal growth of plants.

We ended up varying belowground resource units between 60 and 120 (medium and high resource level) and aboveground resource units between 50 and 100 (medium and high resource level). 90 different resource combinations were selected using Latin Hypercube Sampling (LHS; Iman, 1999), therefore, covering uniformly the sampling space. Each resource combination was repeated ten times to account for stochasticity, resulting in 900 simulation runs.

Species classification into PFTs

We classified the six plant species according to the categories used in Weiß et al. (2014) and Reeg et al. (2017) (Table 2.3). Without any further adaption, the monoculture control biomass of *L. hispidus*, *T. pratense* and *S. nutans* could not be sufficiently predicted by the model. The experimental biomass of *T. pratense* was even higher than the maximal plant masses assumed in the model according to the classification. Also for *L. hispidus* the modelled biomass was not able to increase further due to the maximal plant size assumed in the trait characterization. Thus, we increased the maximal plant mass of these two species to the next higher category (from small to medium sized plant species). This can be also supported by data found in the TRY database for maximal plant size (Kattge et al., 2011). According to the root/shoot ratios found in the trait database (Hicker, 1999; Everwand et al., 2014; Fry et al., 2014) and according to expert knowledge (Michael Ristow, University of Potsdam, Germany, personal communication, 2017), *S. nutans* allocates more resources to root growth compared to other plant species, especially in early live stages (approx. 50% higher root biomass than shoot biomass, Hicker, 1999). In contrast to that, *T. pratense* has

Table 2.3: Classification of species into plant functional types (PFT) according to classification rules (Reeg et al., 2017) and current adaptations. During the calibration process (i.e. fitting simulated shoot growth against empirical shoot growth in monoculture controls) a root/shoot allocation trait was integrated in the model. The trait characteristics are based on trait data ('root/shoot ratio') and expert knowledge.

Species	Plant size	Growth form	Resource response	Grazing response	Root/shoot allocation
B. erectus	Large	Semi-rosette	Stress-tolerator	Tolerator	Alloc_root/shoot = 1
C. cristatus	Large	Semi-rosette	Intermediate	Avoider	Alloc_root/shoot = 1
G. mollugo	Medium	Erect	Competitor	Intermediate	Alloc_root/shoot = 1
L. hispidus	Medium[a]	Rosette	Intermediate	Tolerator	Alloc_root/shoot = 1
S. nutans	Medium	Semi-rosette	Intermediate	Intermediate	Alloc_root = 0.5 Alloc_shoot = 1
T. pratense	Medium[a]	Semi-rosette	Competitor	Tolerator	Alloc_root = 1 Alloc_shoot = 0.2

[a] According to classification rules the species would be classified as small. However, experimental data reach or exceed the maximal plant size even within 6 weeks of growth. Therefore, we classified these species in the next higher category.

higher shoot biomasses (approx. 20%, Everwand et al. 2014; Fry et al. 2014). Based on this knowledge, we integrated a root and shoot allocation factor in the model (Eqs. 2.1a, b; Eqs. 2.2a, b).

Higher resource allocation into the shoot growth was simulated as:

$$\text{shoot\_resources} = \text{shoot\_resources} + (\text{root\_resources} * \text{alloc\_shoot}) \qquad \text{Eq. 2.1a}$$

$$\text{root\_resources} = \text{root\_resources} * (1\text{-alloc\_shoot}) \qquad \text{Eq. 2.1b}$$

Higher resource allocation into the root growth was simulated as:

$$\text{shoot\_resources} = \text{shoot\_resources} * (1\text{-alloc\_root}) \qquad \text{Eq. 2.2a}$$

$$\text{root\_resources} = \text{root\_resources} + (\text{shoot\_resources} * \text{alloc\_root}) \qquad \text{Eq. 2.2b}$$

With *Shoot/Root_resources*: the resources allocated to root and shoot growth without the allocation factor and *alloc_shoot/root*: the PFT-specific allocation factor.

These factors allow for an additional shift in resource allocation from shoots to roots and vice versa after the general distribution of resources between roots and shoots. For *T. pratense*, 20% of the resources assigned for root growth were additionally available and shifted to shoot growth. In the case of *S. nutans*, 50% of the resources assigned for shoot growth were additionally available and shifted to root growth.

Integration of herbicidal effects

The design of the empirical study was based on the OECD Guideline for Vegetative Vigour studies (OECD, 2006b) and focused on the endpoint biomass, not measuring the effect on seedling emergence or survival. This means, plant individuals were oversprayed with different application rates and fresh weight was measured 2, 4 and 6 weeks after application. Therefore, we integrated the herbicide effect in the model only as a reduction in biomass gain per weekly time step.

The herbicide effect was based on the effects on fresh weight (reduction in shoot mass) measured 4 weeks after application in the experimental monocultures. We selected the 4th week to be as close as possible to the standardized greenhouse experiments, which measure effects on biomass 3–4 weeks after herbicide application. For each species and herbicide, the dose–response curves were calculated using an optimization algorithm (Nelder and Mead, 1965), which calculates the *ER50* and slope (*b*) estimates of the dose–response function (Eq. 2.3):

$$\mathit{Effect}(\text{application rate}) = \text{application rate}^{b} / (\text{ER50}^{b} + \text{application rate}^{b}) \qquad \text{Eq. 2.3}$$

Effect is the reduction in growth for the specific application rate, application rate is the applied rate of the herbicide [in g/ha for Monitor® or mL/ha for RoundUp®], *ER50* is the rate [in mL/ha for Monitor® or g/ha for RoundUp®], at which 50% reduction of biomass occurred, and *b* is the slope for the dose–response function. Effect and slope *b* are dimensionless.

In each weekly time step following the simulated herbicide application in the model, the biomass gain was reduced by this species and dose specific effect based on the dose–response data. We assumed no dissipation of the herbicides throughout the time of the experiment, i.e., the effect does not change over time. This holds true for both the modelled monocultures and communities: Modelled effects are based on these species-specific dose responses and applied each week after herbicide application.

Analyses

For model calibration and the comparison of the aboveground biomasses without herbicide effect, we used pattern- oriented modelling—the visual comparison of the patterns (i.e., shoot mass dynamics over time) observed in the empirical data compared to those in the modelled simulations. Therefore, we first needed to convert the empirically measured fresh weights to dry weight, which is the biomass parameter simulated in IBC-grass.

We repeated the control monoculture experiment to measure the fresh to dry weight ratio for each species and used the mean ratio as a conversion factor (see 7.1.2 for further details). Besides pattern-oriented calibration, we calculated the Welch Two Sample t test (not paired, no correction for multiple comparison, alpha value = 0.05) for each experimental and modelled pair (by PFT and time) of data to determine whether significant differences exist (see 7.1.3 for detailed test results).

In addition to the visual comparison of the observed patterns of the predicted and empirically measured effects in the monocultures and communities, we also calculated the model adequacy and model reliability according to Scholten and van der Tol (1994). We calculated the area covered by the 2.5th and 97.5th percentile of the modelled data (*M*, Eq. 2.4) on the one hand and of the empirical data (*O*, Eq. 2.5) on the other hand. In addition, we calculated the area of the intersection of *M* and *O* (*I*, Eq. 2.6).

$$M = \sum_{t=1}^{3} \left|\text{2.5th percentile modelled shoot mass}_{2t} - \text{97.5th percentile modelled shoot mass}_{2t}\right| \quad \text{Eq. 2.4}$$

$$O = \sum_{t=1}^{3} \left|\min(\text{experimental shoot mass}_{2t}) - \max(\text{experimental shoot mass}_{2t})\right| \quad \text{Eq. 2.5}$$

$$I = \sum_{t=1}^{3} \left|\max(\text{2.5th percentile modelled shoot mass}_{2t}, \min(\text{experimental shoot mass})_{2}) - \min(\text{97.5th percentile modelled shoot mass}_{2t}, \max(\text{experimental shoot mass})_{2t})\right| \quad \text{Eq. 2.6}$$

Model adequacy describes which part of the experimental data can be explained by the model. It is calculated by dividing the intersection I with the area of the observed data in the experiments (O) (adequacy = I/O). Model reliability describes which part of the modelled data can also be observed in the experimental data. Therefore, we put the intersection I in relation to the modelled data area M (reliability = I/M). Both endpoints can have values between 0 and 1. If model adequacy is 1, all observed data fall within the range of the modelled data. If model reliability is 1, all modelled data fall within the range of the observed data. Thus, in the best case that both values are 1, there is a complete overlap between modelled and observed data and the model is able to fully represent the empirically observed data. If both the adequacy and reliability have values close to zero, there is almost no overlap between modelled and observed data (i.e., the intersection area I is close to zero).

CALIBRATION RESULTS

CONTROL GROWTH

With the model adjustments mentioned before, we were able to simulate similar biomasses in the control monocultures of the six tested plant species over the 6 weeks (Fig. 2.2) compared to the empirical data. Only for the last measurement in week 6, *C. cristatus* and *L. hispidus* show significant differences. In the experiments, the biomass of *C. cristatus* even decreased without any herbicide effect. The latter might imply an empirical bias, i.e., the growing conditions in the experiment were not suitable for *C. cristatus* and thus plants were impaired in their growth even without any herbicide impact. On the other hand, as we converted the empirically measured fresh weight to dry weight using a species-specific static conversion factor, the potential intraspecific and temporal variability of the fresh to dry weight ratio might be underestimated. Still, there is a high overlap between model and empirical data and on average the simulated shoot weights for the monocultures are on the same level as the empirical effects.

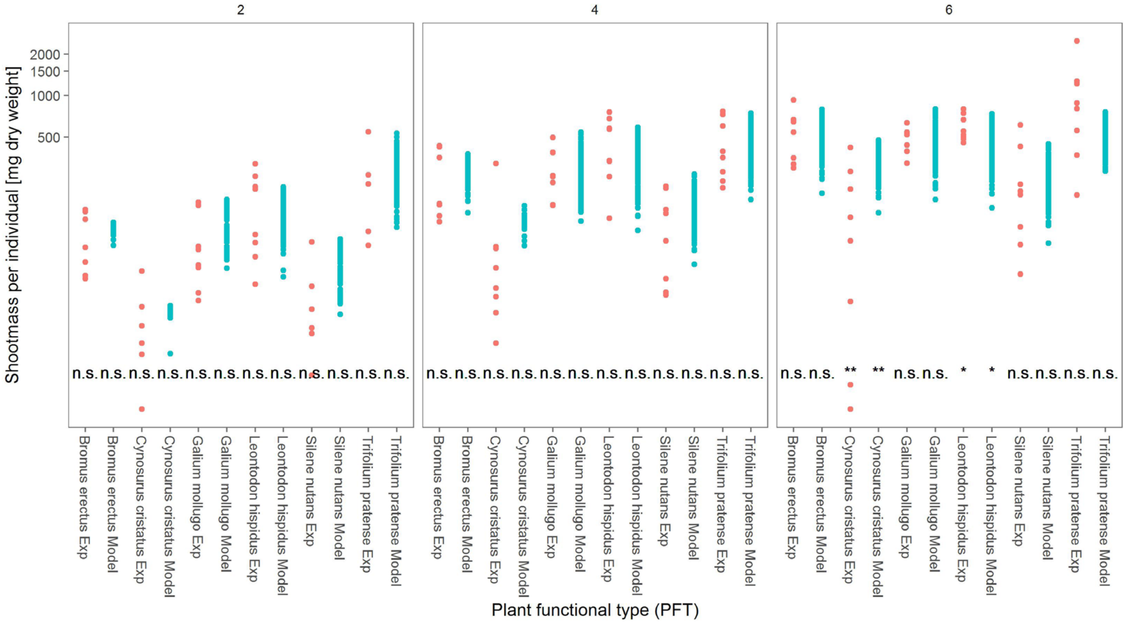

Figure 2.2: Model calibration to empirical monocultures: Comparing the shoot weight of experimentally measured (red points, N = 8) and modelled (blue points, N = 900 covering potential variability in resource levels) data for each assessment date in control monocultures. Experimental values measured in fresh weight were converted to dry weight using a conversion factor based on a repeated monoculture control experiment, in which we measured the fresh to dry weight ratio of each species (see 7.1.2 for further details). Both broad spectrum herbicide and selective herbicide control values are included in the experimental data. Each experiment-model pair was tested for significance using a t-test; not significant results indicate that there are no differences between experimental and model data. Please note the logarithmic scale of the y-axis.

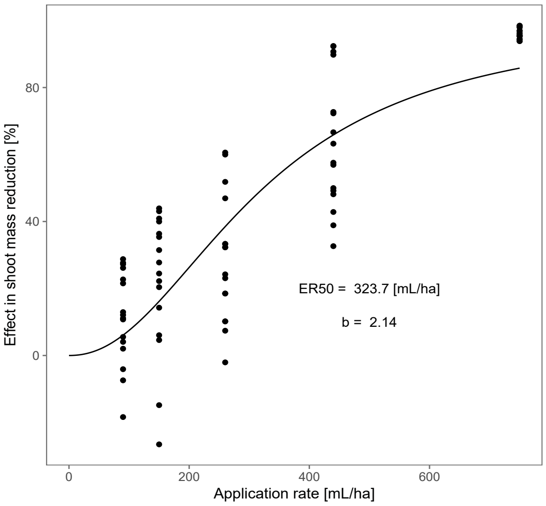

Figure 2.3: Effects on the fresh weight (% reduction of fresh weight) of *B. erectus* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the broad spectrum herbicide RoundUp®. Points show the empirically measured data and the line the estimated dose–response curve based on the dose-response function (Eq. 2.3), with the predictors for the *ER50* value and the slope *b*

HERBICIDAL EFFECTS

We calculated the dose–response function based on the empirical effects measured 4 weeks after application in the monoculture experiment. Table 2.4 summarizes the results of the optimization algorithm and Fig. 2.3 shows an exemplary dose response for *B. erectus* when affected by the broad spectrum herbicide RoundUp® (see 7.1.4 for all dose–response curves). Especially the dose responses of the selective herbicide Monitor® show the different herbicide sensitivities of the test species.

Table 2.4: Estimated *ER50* values and slopes *b* for the 6 test species and the two herbicides including the standard errors (see 7.1.4 for all dose–response curves)

Herbicide	Species	ER50	ER50 error	Slope b	Slope b error
Broad spectrum herbicide RoundUp®	*B. erectus*	323.69	12.5	2.14	0.18
	C. cristatus	94.88	5.88	2.07	0.31
	G. mollugo	104.88	1.62	4.57	0.33
	L. hispidus	111.16	4.47	2.24	0.22
	S. nutans	149.93	12.09	1.46	0.18
	T. pratense	233.5	12.33	1.36	0.11
Selective herbicide Monitor®	*B. erectus*	25.23	7.2	0.64	0.12
	C. cristatus	1.73	0.44	0.67	0.17
	G. mollugo	1.52	0.06	1.93	0.19
	L. hispidus	1.8	0.21	0.86	0.11
	S. nutans	1.68	0.21	0.69	0.08
	T. pratense	4.74	0[a]	-0.08	0[a]

[a] The optimization routine was not able to calculate the Hessian matrix. Therefore, we were not able to calculate an error.

2.4 Results

2.4.1 Prediction of control growth in communities

After calibration, the IBC-grass model was able to predict similar shoot masses in the artificial communities without herbicide effect (i.e., control data, Fig. 2.4). Most of the species-specific comparisons were not significantly different from each other. In the case of *C. cristatus*, the predicted and observed biomasses were significantly different; however, all empirical data are within the range of the model predictions. The good prediction of the control communities is underlined also by high adequacy and reliability values (Table 2.5). All values are above 0.6, except for the model adequacy of *T. pratense*. For this species, only 20% of the modelled shoot masses in the artificial communities are similar to empirically measured values. Nevertheless, the reliability for modelling *T. pratense* in these artificial communities is still 0.6, meaning that 60% of the observed data were predicted by the model.

Table 2.5: Model adequacy and reliability values for the predicted control communities. The values show the mean over all three measurements (weeks 2, 4 and 6). Model adequacy is the intersection of the modelled and empirical data space divided with the observed data space. If the value is 1, all observed data points fall within the modelled area. Model reliability is the intersection divided with the modeled data space. If the value is 1, all modelled data points fall within the observed area

PFT	Adequacy	Reliability
B. erectus	0.67	0.89
C. cristatus	0.79	0.73
G. mollugo	0.82	0.75
L. hispidus	0.62	0.89
S. nutans	0.66	0.79
T. pratense	0.2	0.6

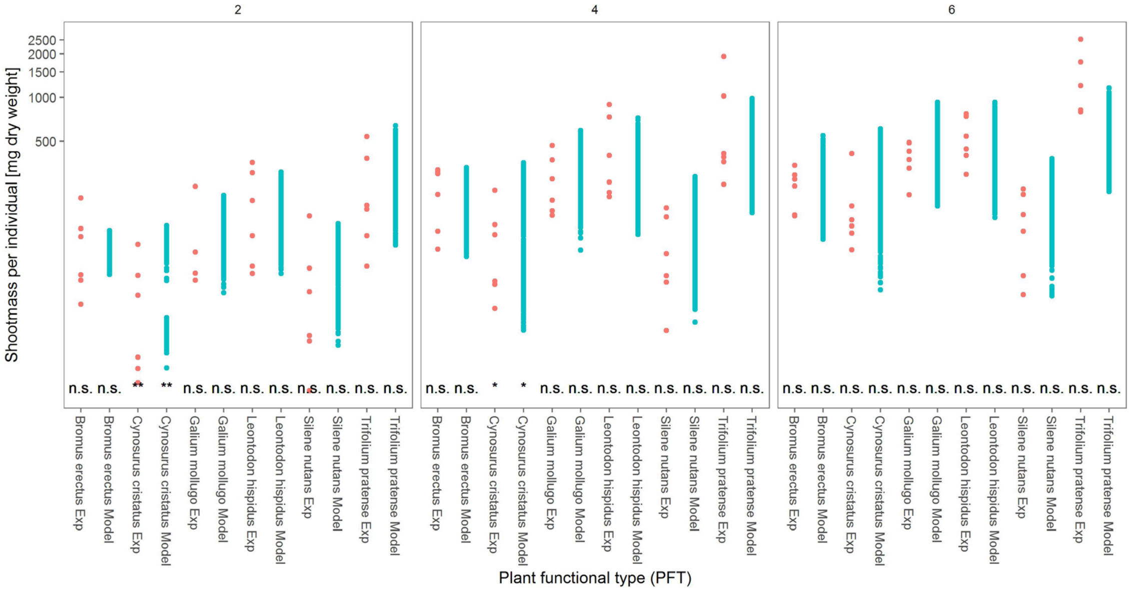

Figure 2.4: Prediction of shoot growth in control community: Comparing the shoot weight of experimentally measured (red points, N = 8) and modelled (blue points, N = 900 covering potential variability in resource levels) data for each assessment date in control communities. Experimental values measured in fresh weight were converted to dry weight using a conversion factor based on a repeated monoculture control experiment, in which we measured the fresh to dry weight ratio of each species. Both broad spectrum herbicide and selective herbicide control values are included in the experimental data. Each experiment-model pair was tested for significance using a t-test; not significant results indicate that there are no differences between experimental and model data. Please note the logarithmic scale of the y-axis.

Table 2.6: Model fit for the monocultures. Mean model adequacy and reliability over all herbicide application rates for the selective and the broad spectrum herbicide. Model adequacy is the intersection of the modelled and empirical data space divided with the observed data space. If the value is 1, all observed data points fall within the modelled area. Model reliability is the intersection divided with the modeled data space. If the value is 1, all modeled data points fall within the observed area

PFT	Selective herbicide		Broad spectrum herbicide	
	Adequacy	Reliability	Adequacy	Reliability
B. erectus	0,46	0,53	0,48	0,63
C. cristatus	0,73	0,52	0,93	0,17
G. mollugo	0,37	0,93	0,41	0,28
L. hispidus	0,55	0,78	0,49	0,43
S. nutans	0,79	0,74	0,67	0,42
T. pratense	0,77	0,86	0,65	0,73
all	0,61	0,73	0,61	0,44

2.4.2 Prediction of herbicide impacts based on monoculture dose responses

MONOCULTURES

In the monoculture treatment, the calibrated IBC-grass model showed a good reliability for both the selective herbicide as well as the broad spectrum herbicide (Table 2.6). In 56–100% of the simulation runs, in which we varied above and belowground resource levels (see Methods, overall 900 simulation runs with 90 different resource level combinations and 10 repetitions for each combination), the predicted effects are within the range of the experimentally measured effects (Fig. 2.5). The observed effects on the shoot masses of the 6 different PFTs over time (i.e., patterns) are comparable to the patterns predicted by the model. For example, for the realistic drift rate of 3.0% of the maximum application rate of the broad spectrum herbicide RoundUp® (≡90 mL/ha), the mean effect on the shoot mass of *B. erectus* remained negligible in both the empirical data as well as in the model predictions. In contrast to that, the mean effects on *C. cristatus* are increasing over time in both the empirical and modelled data. However, especially at this lowest test rate which is similar or slightly higher than the predicted EU drift rate (2.77%), some species show a very high variation in the experiments (e.g., *C. cristatus*). That biological variation is not covered in IBC-grass, which is also reflected in lower model adequacy (Table 2.6). The design of the toxicological submodel, transferring the empirical effects measured in the monocultures 4 weeks after application as a weekly reduction in the biomass gain, results in a good representation of the observed patterns and temporal dynamics of the species-specific effects. Nevertheless, it needs to be kept in mind that the dose responses, on which the individual-level effects are based on in the model, were calculated using the empirical monoculture data 4 weeks after application. Thus, the modelled data are not completely independent from the empirical data.

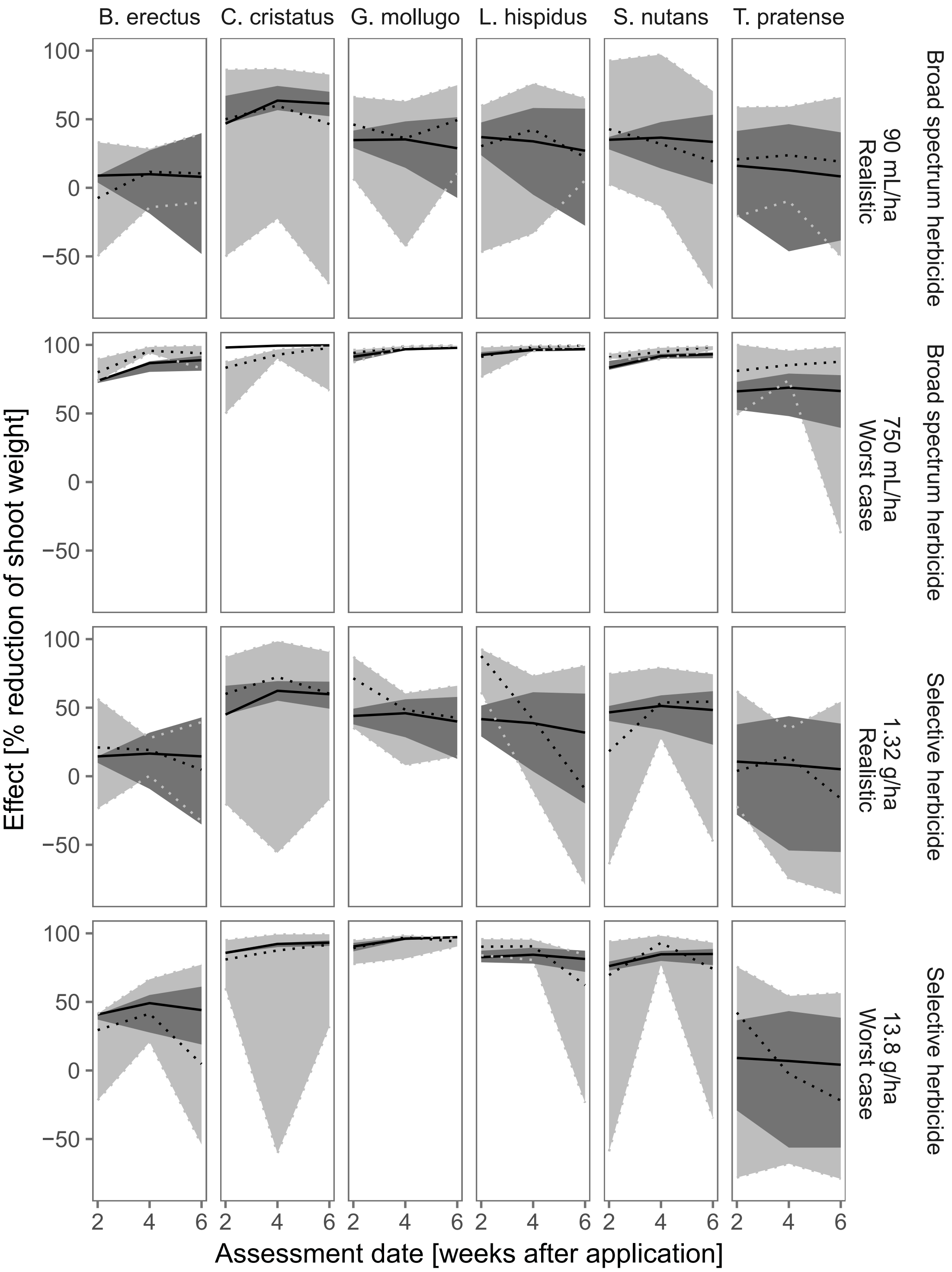

Figure 2.5: Effects on species specific shoot masses (treatment/control) in the monocultures after herbicide application. Black solid lines represent the median of the model predictions and dark gray ribbons show the upper and lower 2.5th percentile of the predictions. Dotted black lines show the empirically measured median and gray ribbons and dotted gray lines the upper and lower 2.5th percentile of these. Only the lowest (realistic) and highest (worst-case) tested application rates are presented here. The lowest rates tested were in the same range (broad spectrum herbicide RoundUp®) or higher (selective herbicide Monitor®) than the rates that would be applicable to the risk assessment considering European standard drift rates. The results for these test rates are presented to deliver a more realistic picture. Results for the whole range of tested application rates can be found in 7.1.5.

ARTIFICIAL COMMUNITIES

In general, the predicted temporal patterns and magnitude of the effects on plant populations in an artificial community of the model IBC-grass are comparable to the observed patterns and magnitude (Fig. 2.6). Model adequacy is higher than in the monocultures (Table 2.7, compared to Table 2.6). The variation in the simulated communities is greater than that in the monocultures due to the additional interspecific competition. Therefore, the model is able to cover the natural variability found in the experiments to a greater extent. There are slight differences between the two herbicides (selective and broad spectrum herbicide), but looking at all plant species (or PFTs), the adequacy is the same. Model reliability is smaller than in the monocultures, especially for the broad spectrum herbicide, meaning that a lower percentage of the model predictions is within the range of observed effects (Fig. 2.6). This can be explained by a higher variability in the predicted effects due to interspecific competition between plant individuals (compared to the monocultures).

Table 2.7:Model fit for the communities. Mean model adequacy and reliability over all herbicide application rates of the selective (Monitor®) and the broad spectrum herbicide (RoundUp®). Model adequacy is the intersection of the modeled and empirical data space divided with the observed data space. If the value is 1, all observed data points fall within the modeled area. Model reliability is the intersection divided with the modeled data space. If the value is 1, all modeled data points fall within the observed area

PFT	Selective herbicide		Broad spectrum herbicide	
	Adequacy	Reliability	Adequacy	Reliability
B. erectus	0,46	0,53	0,48	0,63
C. cristatus	0,73	0,52	0,93	0,17
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T. pratense	0,77	0,86	0,65	0,73
all	0,61	0,73	0,61	0,44

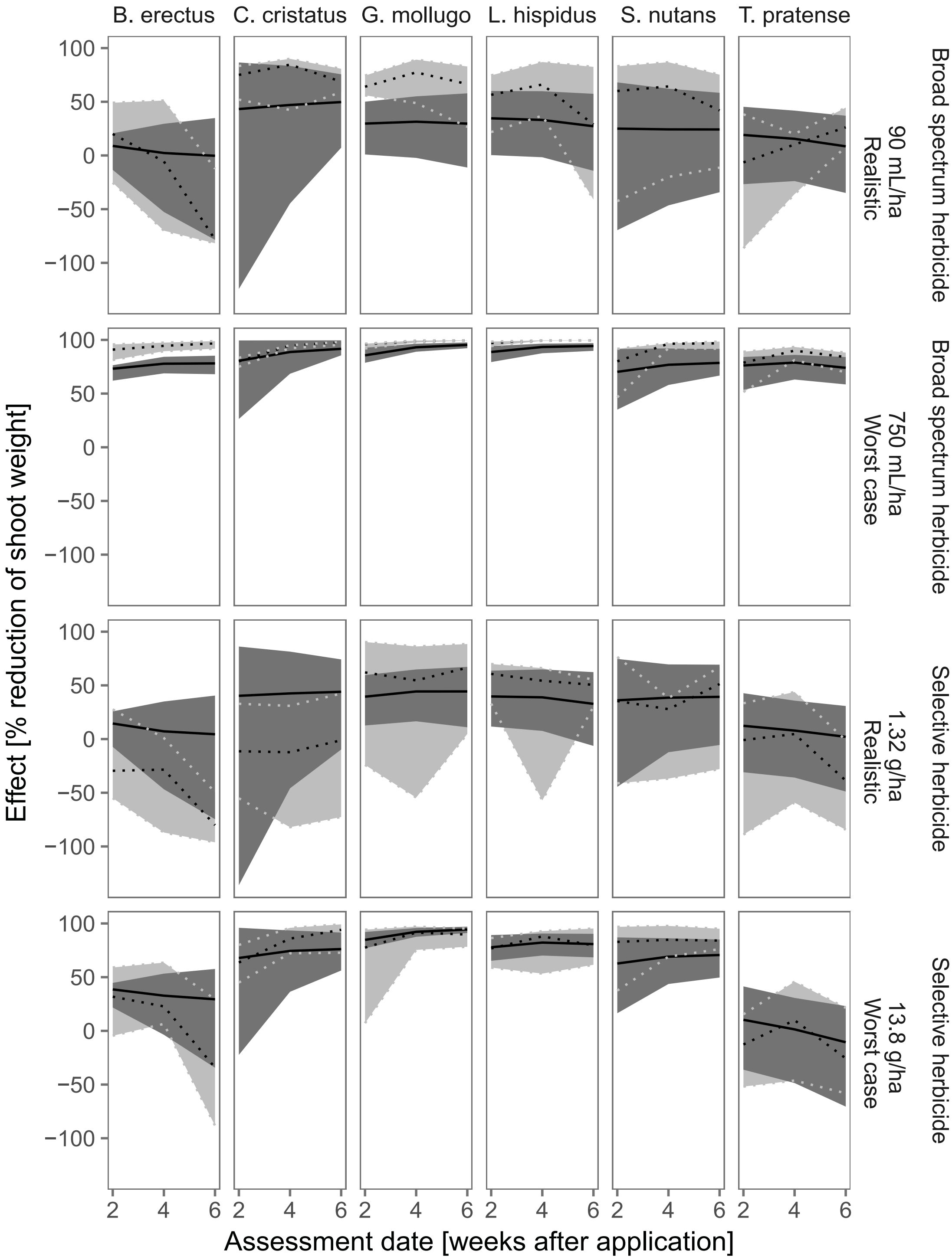

Figure 2.6: Effects on species specific shoot masses (treatment/control) in the artificial communities after herbicide application. Black solid lines represent the median of the model predictions and dark gray ribbons show the upper and lower 2.5th percentile of the predictions. Dotted black lines show the empirically measured median and gray ribbons and dotted gray lines the upper and lower 2.5th percentile of these. Only the lowest (realistic) and highest (worst-case) tested application rates are presented here. The lowest rates tested were in the same range (broad spectrum herbicide RoundUp®) or higher (selective herbicide Monitor®) than the rates that would be applicable to the risk assessment considering European standard drift rates. The results for these test rates are presented to deliver a more realistic picture. Results for the whole range of tested application rates can be found in 7.1.5

2.5 Discussion

In a plant community, inter- and intraspecific competition plays a major role in determining the dynamics within the community. Thus, indirect impacts of herbicides on populations as well as on plant community dynamics might appear, especially if affected plants differ in their susceptibility (e.g., if selective herbicides are applied). As a result, the competitive relationship between plant individuals in a community might shift between individuals of different plant species and, consequently, indirect impacts might alter plant community dynamics (see, e.g., Reeg et al., 2017). Such indirect effects on plant species not impaired by the herbicide were observed in the study of Reuter and Siemoneit-Gast (2007), especially regarding the selective herbicide Monitor®. Already in this short-term study, for instance the shoot mass of *T. pratense*, being less sensitive to the herbicide than other test species, increased due to lower interspecific competition from more sensitive plant species such as *G. mollugo* with a decreasing shoot mass. After the calibration process, where the IBC-grass model was solely adapted to the monoculture control data of the experiment (Reuter and Siemoneit-Gast, 2007), the model was able to not only predict shoot masses measured in control communities without further model adaptations, but also to predict similar effect intensities and dynamics over time in these artificial communities. Similar to the empirical results, *T. pratense* showed only minor decreases in shoot masses or even an increase under herbicide treatments; whereas for *G. mollugo* the model predicted a high negative impact on the shoot mass.

The study setup allows us to make conclusions about the intra- as well as interspecific competition and their reflection in the model: in monocultures, only plant individuals of the same species compete for resources and space, whereas in the artificial communities both types of competition occur: between individuals of the same species and between individuals of different species. Although we did not quantify the specific impact of intra- or interspecific competition in the empirical data, it can be assumed that competition occurs as soon as plant individuals overlap in their roots or shoots. As the distance between the plant individuals is quite small (2.5 cm), an overlap of roots and shoots is very likely. We were able to calibrate the model to the monoculture control growth, where only intraspecific competition took place. This allows the conclusion that the intraspecific competition is indeed well reflected in the model. The fact that we did not touch any process regarding the competition during the calibration process even strengthens this conclusion. Excluding the competition from this calibrated model actually showed that simulated plant growth would have exceeded the empirical measurements (see 7.1.6). Also interspecific competition is well reflected in the model: On the one hand, the model predicted similar shoot masses in control communities. The main difference compared to the monoculture simulation is actually the interspecific competition process. And, on the other hand, also similar effect intensities and temporal dynamics under herbicide treatment were predicted. Thus, indirect effects resulting from intraspecific competition due to the different species specific susceptibilities are reflected by the model.

Furthermore, the model was able to predict similar short-term herbicide impacts on communities based on the species specific dose responses (calculated from empirical effects in monocultures measured 4 weeks after application) compared to empirical data. The guidance document currently in use in the EU specifies an assessment factor, which is supposed to cover the uncertainties in the risk assessment for non-target terrestrial plants, e.g., the extrapolation from individual-level tests to the community level or the occurrence of even more sensitive species (EC, 2002). However, the appropriateness of the assessment factor for covering uncertainties is debated. Participants of a non-target terrestrial plant workshops held by the Society of Environmental Toxicology and Chemistry (SETAC) in 2014 and 2015 recommended using modelling approaches to support the risk assessment of terrestrial plant communities (Arts et al., 2017). The current study strengthens that the presented plant community model IBC-grass is suitable to be used for analysing short-term effects on a plant community based on monoculture dose responses, which can be derived from the standard studies used for the current non-target terrestrial plant risk assessment. However, also the extrapolation from short-term to long-term effects is important to estimate the potential risk on non-target terrestrial plant communities. Therefore, longer term field data are required to evaluate the models' accuracy and reliability for predicting long-term impacts of herbicides and therewith strengthen the model's credibility for risk assessors. It would be valuable if new empirical studies were designed to be used as additional data for validating ecological models like IBC-grass, e.g., measuring biomass on individual level over a longer time period.

Plant communities show a high natural variability. This variability is caused by various factors, e.g., heterogeneity in the soil (i.e., in nutrients or moisture) or aboveground and belowground disturbances by grazing, trampling or management practices, but also the history of the landscape is important for its current state. To adequately characterize herbicide-related effects on plant communities, a high amount of replication is needed. Thus, the field studies are not only labour and cost intensive but also put high demands on the study site, e.g., a large homogeneous field area in order to disentangle the herbicide impact from other factors determining the variability. Ecological models can overcome this dilemma if they comprise the main drivers for the variability in plant community dynamics, which were mentioned earlier. Different scenarios (e.g., resource levels, management practices) can be simulated to cover for various conditions occurring in semi-natural grasslands. In IBC-grass indeed many of these factors are included: resource levels and disturbances such as grazing, trampling and cutting are integrated in the model. As previous studies showed, the IBC-grass model is able to predict also long-term impacts on grassland communities. For example, Weiß et al. (2014) analysed the effect of different grazing intensities and realistically predicted the yield under different grazing regimes. Integrating resource heterogeneity directly in the model might be desirable for improving the model performance. However, heterogeneity in resources can also be covered by simulating small plots with a variety of potential resource levels similar to sample sub-plots in empirical studies to cover the natural variability, which is comparable to the approach in the current study.

As several environmental parameters (e.g., resource levels, disturbances, PFT pool) can be changed in IBC-grass, different environments can be covered. However, the model was originally developed and validated for semi-natural grasslands in Germany. Therefore, special environmental conditions, e.g., occurring in drylands or wetlands, which are driven or limited by other factors such as soil moisture, fire or salinity, are currently not covered in the model. Thus, the processes driving these specific ecosystems would need to be integrated in the model beforehand in order to be suitable for the corresponding risk assessments. However, for semi-natural grasslands in regions, which have similar environmental conditions to German grasslands, IBC-grass can provide reasonable assessments of potential outcomes of herbicide impacts on community level (see Reeg et al., 2017 for potential long-term effects of herbicide impacts on different grassland communities occurring adjacent to agricultural fields in Germany).

To evaluate the credibility of model predictions using empirical data, we chose to calculate model adequacy and reliability (Scholten and Van der Tol, 1994). Both values are equally important to qualify the model predictions. Reliability explains which part of the model predictions is observed in the empirical data. Thus, it is a measure to estimate in how many simulations the model is in agreement with empirical data. Adequacy, on the other hand explains which part of the observed data is predicted. It gives an idea whether the model is covering also the extreme cases, e.g., the strongest effects that were observed. Therefore, both measurements should always be reported and considered in combination. For example, if all model predictions have also been observed, but only cover a small range of the variability in the observed data, the reliability is high; however, the adequacy is low. Ideally, you would want to have a high adequacy and a high reliability. In general, it is important to be aware of the instances which might not be covered by the model.

With the detailed model description following the ODD protocol (Reeg et al., 2017), sensitivity analyses (Weiß et al., 2014; Reeg et al., 2018a) and the short-term validation in the current study, IBC-grass now fulfils the main aspects for an ecological model to be used for ecological risk assessments and thus for environmental decision making (Schmolke et al., 2010). Based on individual-level effects measured in standard greenhouse experiments, IBC-grass can extrapolate the effects up to community level. Thus, a range of different environmental scenarios and the effect on different grassland communities can be simulated to estimate the potential risk posed by herbicide applications on non-target terrestrial plants. The current study showed that for short-term effects the model is realistically predicting the community-level effects. To strengthen the credibility of the model also for long-term effects, a validation based on long-term effect data is desirable; however, it is difficult to reach as there is a lack of suitable long-term field studies.

2.6 Conclusions

In this current study, we were able to show that the plant community model IBC-grass was able to realistically predict short-term community-level effects on plant biomass based on monoculture dose–response data. It represents an approach how individual-level effects measured in current standard greenhouse experiments can be integrated in a community model to estimate community-level effects in ecological risk assessments of herbicides. Such validated plant community models might be especially important in the future as EFSA considers specific protection goals for non-target terrestrial plants on population and community level (EFSA PPR Panel, 2014a).

3 Potential impact of effects on reproductive attributes induced by herbicides on a plant community[1]

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[1] published as: Reeg J, Heine S, Mihan C, Preuss TG, McGee S, Jeltsch F. 2018. Potential impact of effects on reproductive attributes induced by herbicides on a plant community. Environ Toxicol Chem. 37(6):1707-1722. DOI: 10.1002/etc.4122. This article may be used for non-commercial purposes in accordance with Wiley Terms and Conditions for Use of Self-Archived Versions.

3.1 Abstract

Current herbicide risk assessment guidelines for non-target terrestrial plants require testing effects on young, vulnerable life stages (i.e., seedling emergence [and subsequent growth] and vegetative vigour [growth and dry wt]) but not directly on the reproduction of plants. However, the European Food Safety Authority (EFSA) has proposed that effects on reproduction might be considered when evaluating the potential effects on plants. We adapted the plant community model for grassland (IBC-grass) to give insight into the current debate on the sensitivity of reproductive versus vegetative endpoints in ecological risk assessment. In an extensive sensitivity analysis of this model, we compared plant attributes potentially affected by herbicides and the consequences for long-term plant population dynamics and plant diversity. This evaluation was implemented by reducing reproductive as well as vegetative endpoints by certain percentages (e.g., 10–90%) as a theoretical assumption. Plant mortality and seed sterility (i.e., inability of seeds to germinate) were the most sensitive attributes. Our results indicated that effects on seed production at off-field exposure rates must be very strong to have an impact on the risk assessment. Otherwise, effects on seed production are compensated for by the soil seed bank. The present study highlights the usefulness of community level modelling studies to support regulators in their decisions on the appropriate risk assessment endpoints and provides confidence in their assessments.

3.2 Introduction

Weeds are undesired plant species in a particular environment. In agricultural fields, weeds are plant species that compete with crop species and often lead to reduced yields of up to 30% (Bagg et al., 2017). To maintain crop health and yields, weeds must be controlled within fields. Various methods may be available for this (e.g., mechanical weeding, thermal or chemical weed control; Bagg et al., 2017), depending on the agricultural practices, labour, and technology available. In conventional intensive agriculture, chemical weed control via herbicides is the most practical and common method applied. With different modes of action, herbicides affect the growth and survival of target plant species. Herbicides may target all non-crop species in an agricultural field (in-field) or specific monocotyledonous or dicotyledonous plant species. Outside the agricultural field (off-field), in the field boundary and direct neighbourhood of an agricultural field, these species are considered non-target and therefore exposure to herbicides should be limited to conserve semi-natural plant communities. Nevertheless, a combination of certain situations such as weather conditions, application methods, and landscape structure might result in the drift of low doses of herbicides into these off-field areas. According to the Environmental Risk Assessment Scheme, these potentially occurring risks need to be mitigated by buffer zones or drift reduction technology (EPPO, 2003).

To identify these risks, the toxicological sensitivity of plants, that is, the impact of a specific herbicide on individual plants, must be evaluated and conclusions need to be drawn on appropriate application patterns that are predicted to not cause unreasonable harm to off-field non-target plants. The Organisation for Economic Co-operation and Development (OECD) and the US Environmental Protection Agency (USEPA) have developed standardized greenhouse experiments—required by regulatory authorities worldwide to characterize the toxicological sensitivity of non-target plants—that can be employed to define herbicide uses safe for non-target plant populations. In these experiments, the potential effects on plant biomass, shoot length, survival, phytotoxicity, and seedling emergence (vegetative vigour test and seedling emergence test, OECD 2006a, 2006b; US EPA 2012a, 2012b, 2012c) are assessed after a herbicide product is applied to the young, vulnerable plants or to the soil surface.

In a deterministic risk assessment scheme, the toxicologically most sensitive endpoint from the seedling emergence and the vegetative vigour tests (i.e., lowest effect rate that was derived for emergence, survival, plant weight, or shoot length) are considered when evaluating the necessity of mitigation measures. If herbicide rates predicted for off-field non-target areas are lower than the toxicologically most sensitive effect rate value that is combined with an assessment factor to cover uncertainties, it is assumed that the herbicide will not have significant effects on non-target terrestrial plants, thus protecting off-field plant populations and communities.

The current OECD and USEPA guidelines do not require endpoints that directly measure the reproduction of plants, for example, seed number or fertility of those seeds. However, the European Food Safety Authority (EFSA) recently proposed that effects on reproduction might be considered when evaluating the potential effects on plant populations (EFSA PPR Panel, 2014a), especially for plant species whose population dynamics rely on seed production. If there is a high seed loss or produced seeds are not fertile, plant populations might decline and eventually become extinct. There are several experimental studies investigating herbicide effects on reproduction and comparing them with vegetative endpoints; however, no general agreement has been reached on a higher or lower toxicological sensitivity of reproductive endpoints, that is, whether the effect rate values for reproductive endpoints are lower than those for vegetative endpoints. Boutin et al. (2014)

summarized 3 different ways that herbicides might potentially impact plant reproduction: 1) plant individuals might show a delayed effect on seed production if they are sprayed at earlier stages (e.g., seedling stage), 2) plant individuals at reproduction stage during spray might show a decrease in seed production, or 3) F1 generation might be affected after the mother plant has been sprayed. In an earlier study, Boutin et al. (2000) tested the first 2 pathways and sprayed multiple plant species at different growth stages. When sprayed in the cotyledon and 2 true-leaf stage (this is the guideline-recommended stage for standard vegetative vigour tests), all tested species showed stronger effects on the vegetative vigour than when sprayed at a later stage. Nonetheless, if plants were sprayed during flower bud or at the onset of flowering, effects on reproductive growth and success were more pronounced, supporting the importance of the plants' stage during herbicide application. Other researchers who compared reproductive endpoints (as a measure of reproductive success) and short- as well as long-term vegetative endpoints concluded that the individual level sensitivity of reproductive endpoints is species- and compound-dependent (Riemens et al., 2008: glufosinate ammonium influenced seed production in *Stellaria media*, but had no effects on seed size if plants are sprayed at an early stage; Riemens et al., 2009: 3 out of 6 plants sprayed with tepraloxydim showed lower sensitivity of reproductive endpoints; Carpenter et al., 2013: 3 out of 5 plants showed effects on long-term reproduction). Overall, these ambiguous results suggest that further research is needed to assess the importance of reproductive endpoints in the framework of registration and regulation of herbicides.

As a further challenge, there is still a lack of knowledge concerning the ecological relevance of individual level endpoints for plant populations and communities over the long term. The EFSA (2010) stated that important protection goals are on the level of functional groups, populations, and communities. Although adverse effects may be observed in single individuals in a guideline study, they have the potential to recover over time (as shown in Carpenter and Boutin, 2010) or to be compensated by a persistent seed bank or seed dispersal if regarded from a population point of view. Accordingly, it is necessary to increase the knowledge of long-term effects on populations and communities (Barnthouse, 2004; Carpenter and Boutin, 2010).

Ecological models are well-established tools to analyse long-term dynamics that can often not be investigated in experimental studies (Shugart, 1989). In our approach, we adapted the spatially explicit, individual-based plant community model for grasslands (IBC-grass; May et al., 2009; Weiß et al., 2014; Reeg et al., 2017) to compare herbicide-induced effects on vegetative vigour and plant survival with effects on reproduction (seed sterility, establishment, and seed production) and their consequences for long-term plant population dynamics and plant diversity. Because the IBC-grass model is an individual-based model, it is well suited to transfer the individual level effects to plant population and community level. In addition, it applies the trait-based approach, that is, classifying plant species into plant functional types (PFTs) with similar trait characteristics; this is supported by the EFSA because PFTs are suitable to link plant diversity to ecosystem processes (Díaz and Cabido, 2001; EFSA PPR Panel, 2014a).

With this modelling approach, we compare the consequences of herbicide-induced effects on reproductive and vegetative endpoints on long-term population and community dynamics. Furthermore, we aim to give insight into the ecological relevance of the current risk assessment scheme based on vegetative endpoints.

3.3 Materials and methods

3.3.1 IBC-grass

As noted previously, IBC-grass is a spatially explicit, individual-based plant community model. Main drivers such as interspecific and intraspecific competition for resources and space as well as disturbances such as grazing, trampling, and mowing are taken into account to reproduce/simulate natural plant community dynamics. The first version of this model was published by May et al. (2009), and was further developed by several researchers (Körner et al., 2014; Weiß et al., 2014). The model version presented in the present study is based on the one described in Reeg et al. (2017). Because of modifications in the above- and below-ground resource levels, the disturbances, and the species pool, the model can be also applied for field boundaries. Additional modifications were performed in the herbicide effect submodel. A detailed model description adhering to the overview, design concepts, and details protocol (Grimm et al., 2006, 2010) can be found in 7.2.1. In the following paragraphs, we will provide a short summary of the main principles, processes, and functions of IBC-grass and a detailed explanation of the modified herbicide effect model.

3.3.2 Main principles

TRAIT-BASED APPROACH

The concept of functional types is often used to explain ecosystem functioning and dynamics (Gross et al., 2017). Species with similar trait characteristics are expected to respond in a similar way to abiotic and biotic conditions. Therefore, these species can be summarized in one PFT. As a result, general processes and dynamics can be simulated for a specific grassland community, whereas still allowing conclusions for other grassland communities with different species but similar PFT composition. In IBC-grass, important traits and trait syndromes (i.e., a set of correlated traits) for grassland dynamics are selected (see Table 3.1 for an overview of the selected traits). Based on the grassland community of interest, species occurring in this community are classified into PFTs according to their trait characteristics. The trait databases BiolFlor, LEDA, and cloPla3 are used to collect the specific trait characteristics (Klotz et al., 2002; Kleyer et al., 2008; Klimésova and de Bello, 2009). The species composition is based on an extensive literature review by K. Bergholz (University of Potsdam, Potsdam, Germany, unpublished data) on herbaceous field boundaries in Europe (see Table 3.2 for community characteristics). In this model version we distinguish between monocotyledonous and dicotyledonous PFTs accounting for selective herbicides (see text under Species-specific susceptibilities heading in Materials and Methods section). The classification into monocotyledonous and dicotyledonous PFTs only relates to herbicide susceptibility and does not involve other trait characteristics. An overview of the plant species and their classification to a specific PFT (with a specific PFT ID) can be found in 7.2.2. The PFT ID is composed of the 4 trait syndromes: plant size (small [S], medium [M], and large [L]), growth form (erect [E], semi-rosette [S], and rosette [R]), resource response type (competitor [C], stress-tolerator [S], and intermediate [I]), and grazing response type (tolerator [T], avoider [A], and intermediate [I]); the clonal type (aclonal, short internodes with resource sharing [cl1], short internodes without resource sharing [cl2], long internodes with resource sharing [cl3], and long internodes without resource sharing [cl4]); and cotyledon characteristic (monocotyledonous [m] and dicotyledonous [d]). For each PFT group, we give an example of a plant species belonging to that group. The characteristics of each PFT ID and the associated plant species can be found in 7.2.2.

Table 3.1: Trait syndromes, plant functional type-specific trait parameter values, and databases used.

Trait/trait syndrome and attributes	Trait parameters				Database
Growth form	f_{leaf}				BiolFlor- rosette attribute
Rosette	1				rosette
Intermediate	0.75				Semi-rosette
Erect	0.5				erect
Maximum plant size	m_{max}	m_{seed}	$mean_{disp}$	std_{disp}	LEDA - seed releasing height
Large	5000 mg	1 mg	0.1 m	0.1 m	>0.87m
Medium	2000 mg	0.3 mg	0.3 m	0.3 m	0.42-0.87m
Small	1000 mg	0.1 mg	0.6 m	0.6 m	<0.42m
Resource response	ru_{max}	$surv_{max}$			BiolFlor - plant strategy type
Competitor	60 resource units	2 wk			c. cr
Intermediate	40 resource units	4 wk			csr. r
Stress-tolerator	20 resource units	6 wk			sr. cs. s
Grazing response	palat	cshoot			BiolFlor – indicator values grazing tolerance
Tolerator	1	1			4-6
Intermediate	0.5	0.75			1-3
Avoider	0.25	0.5			7-9
Herbicide susceptibility	Sens 0-1				Randomly distributed
Clonal integration	Resshare				cloPla3 – persistence of connection
Integrator	1				>=2 years
Splitter	0				<2 years
Lateral spread	SpacerL	stdSpacerL			cloPla3 – lateral spread
Short	2.5 cm	2.5 cm			<0.01 m/y
Long	17.5 cm	12.5 cm			0.01-0.25 m/y and longer

Palat - palatability; Sens - sensitivity; Resshare - resource sharing between spacer.

Table 3.2: Summary of abiotic parameters of the simulated plant community[a]

	Field boundary community
Belowground resources	High
Disturbances	
Cutting per year [at 500mg dw/cm^2]	1
Trampling [% area/year]	10%

[a] The community is based on a literature review by K. Bergholz, University of Potsdam, Germany, unpublished data

2-LAYER ZONE-OF-INFLUENCE APPROACH

The IBC-grass simulates competition between plant individuals via the zone-of-influence approach—distinguishing between above ground and below ground. Individuals are assumed to acquire resources in an area around their location—their zone of influence. If zones of influence of neighbouring individuals overlap, they compete for resources (and space). In IBC-grass, the zone of influence is modelled as a circular area around the stem of an individual. Above ground, the size of the area is determined by the shoot geometry (e.g., rosette) and the shoot mass/size. Above ground the plants compete for light. Competition is simulated partially size-asymmetrically in the way that taller plants acquire more light resources proportional to their shoot mass and geometry. Below ground, it is assumed that the roots of the plants have similar growth forms. Therefore, the below-ground zone of influence depends only on the root mass, that is, high root mass results in a larger zone of influence. In this compartment, competition for resources in overlapping zones of influence is simulated size-symmetrically (i.e., competition is independent of the root size/mass and actual zone of influence).

Spatial dimensions and main state variables

Community dynamics are simulated on a local patch of approximately 3 m^2. This patch is divided into smaller grid cells of 173 x 173 cells of 1 cm^2 each. Each grid cell can contain the stem of 1 plant individual and several seeds. The main state variables are the location (x coordinate, y coordinate), the current shoot, root, and reproductive mass, and the resulting zone of influence of a plant individual, and the location x coordinate and y coordinate of a seed. Periodic boundaries are simulated to avoid edge effects. The local patch is similar to a torus, that is, the edges to the left and right as well as upper and lower edges are connected.

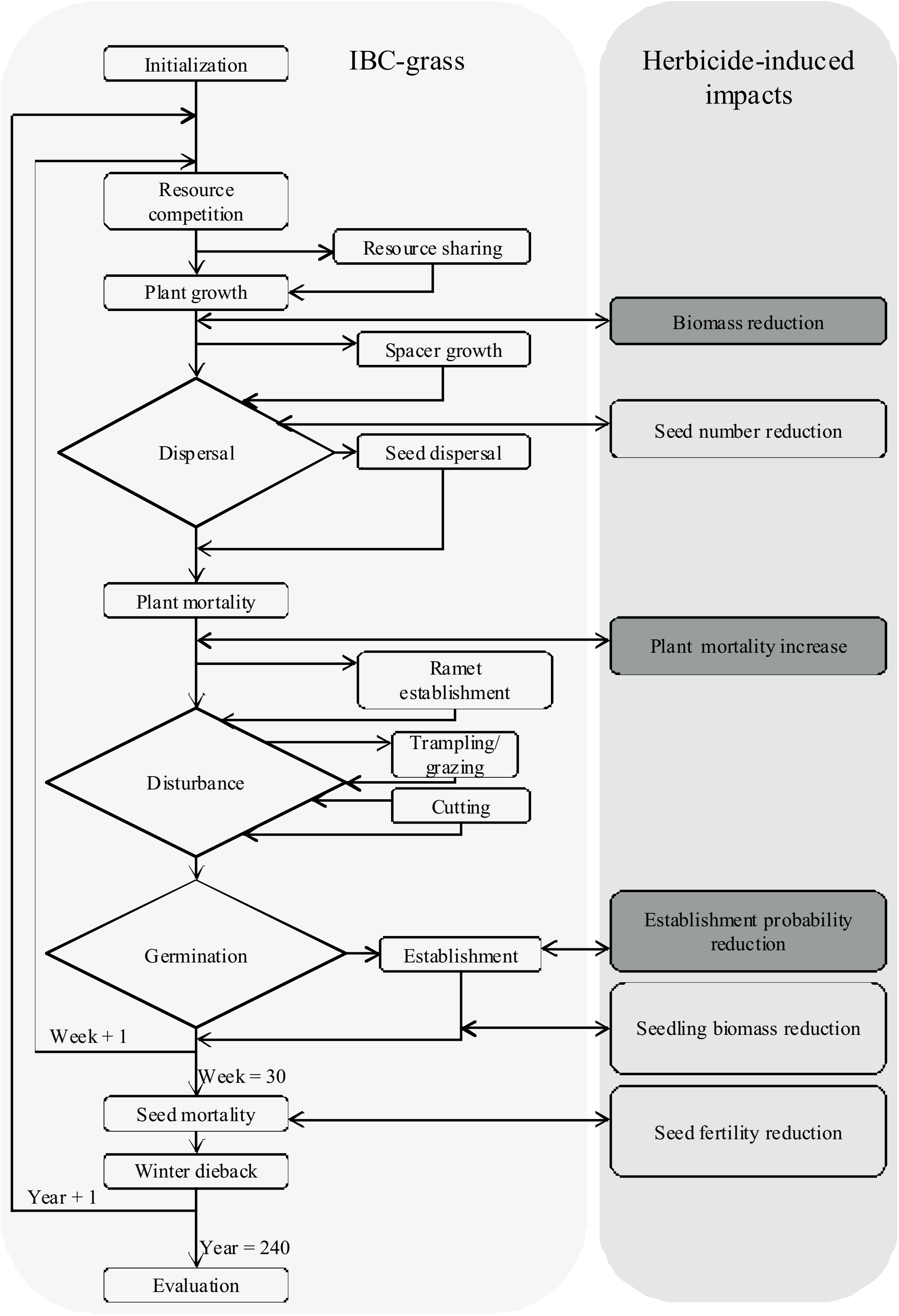

Figure 3.1: Overview and chronology of the main processes in individual-based plant community model for grasslands (IBC-grass) including herbicideinduced impacts. Dark gray boxes mark plant attributes currently tested in ecotoxicological standard tests.

3.3.3 Main processes

The schedule of the main processes is presented in a flowchart (Figure 3.1). In the following paragraphs,we will give a short summary of these processes including the main equations. For a detailed explanation see 7.2.1.

INTERACTIONS AND GROWTH

Plant individuals acquire resources, Δres, in their zones of influence. In areas of overlapping zones of influence they compete for resources (see paragraph introduced by 2-layer zone-of-influence approach in *Materials and Methods* section), with intraspecific competition being stronger than interspecific competition (for details see the overview, design concepts, and details protocol, 7.2.1). The acquired resources are allocated to roots and shoots and converted into biomass based on the constant conversion rate g, the current shoot (root) mass $m_{shoot(root)}$, the trait characteristics of the shoot (root) *cshoot* (*RAR*), the growth form f_{leaf}, the maximal resource utilization ru_{max}, and the maximal plant mass m_{max}. In the absence of competition, this growth function results in a sigmoid growth (Table 3.3, shoot/root growth Equation; see also DeAngelis and Mooij, 2005; Berger et al., 2008). Clonal PFTs invest 5% of their acquired resources in the growth of one spacer (rhizome or

Table 3.3:Main equations in the individual-based plant community model for grasslands regarding competition, growth, and mortality[a]

Process	Equation	Variables
Zone of influence (ZOI)	$A_{shoot} = c_{shoot} * (f_{leaf} * m_{shoot})^{2/3}$ $A_{root} = RAR * m_{root}^{2/3}$	c_{shoot} – PFT specific leaf area RAR – root form (1) f_{leaf} – PFT specific growth form
resource competition	$\Delta res_i = (\beta_i / \Sigma^n{}_{j=1} \beta_j) * Res_{cell}$	$ms_{hoot/root}$ – shoot/root mass [mg dry weight]
asymmetric competition	$\beta_i = ru_{max} * m_{shoot} * f_{leaf}^{-1}$	Res_{cell} – resources in cell ru_{max} – PFT specific maximal resource utilisation
symmetric competition	$\beta_i = ru_{max} * (1/\sqrt{n_{PFT}})$	g – conversion rate resources to biomass
shoot growth	$\Delta m = g * (\Delta res - c_{shoot} * f_{leaf}^{2/3} * ru_{max} * (m_{shoot}^2 / m_{max}^{4/3}))$	n_{PFT} – number of neighbouring PFTs
root growth	$\Delta m = g * (\Delta res - RAR * ru_{max} * (m_{root}^2 / m_{max}^{4/3}))$	m_{max} – PFT specific maximal plant mass [mg dry weight]
density dependent mortality	$p_{mort} = p_{base\_new} + (w_{stress} / surv_{max})$ $p_{base\_new} = p_{base} * (1 + e^{(5 * current\_abundance / max\_abundance)})$	w_{stress} consecutive weeks under stress $surv_{max}$ - PFT specific maximal survival under stress [weeks] p_{base} – base mortality (0.7%) current_abundance – current abundance of a PFT max_abundance – maximal potential abundance of a PFT (assuming fully grown individuals)

[a] More details can be found in the Materials and Methods section and the ODD protocol in Supplemental Data A. ODD = overview, design concepts, and details protocol; PFT = plant functional type.

stolon connecting ramets of clonal plants) per time. The direction of the growing spacer is drawn randomly from a uniform distribution and the distance until establishment is randomly chosen from a normal distribution based on the PFT-specific mean spacer distance (SpacerL; Table 3.1). If the spacer reaches its maximal distance, spacer growth stops and the new ramet establishes with a constant probability pram of 50% if the current cell is not the location of the stem of another plant individual. If the current cell is occupied, the spacer can continue to grow within a radius of 2 cells. If the ramet is established, a new spacer is developed. Therefore, the lateral growth of clonal PFTs is not limited.

MORTALITY

Plant individuals can die as a result of resource stress, random density-dependent mortality, and winter dieback. The probability of death caused by resource stress increases with the duration of resource stress and depends on the characteristics of the trait w_{stress}, which is the maximal number of consecutive weeks of resource stress the plant is able to withstand; that is, the closer the plant individuals get to their maximum survival time under resource stress (i.e., lack of resources to maintain base metabolism), the higher their mortality probability. The basic background mortality of 0.7% corresponds to an annual mortality of 20% (Schippers et al., 2001). It escalates exponentially with increasing population size of the specific PFT to account for density-dependent impacts (e.g., diseases and pests; Reynolds et al., 2003; Bell et al., 2006). During winter, above-ground biomass is decreased by 50% to account for winter dieback. If the resulting biomass is below 10 mg, the plant is considered dead (May et al., 2009; Körner et al., 2014; Weiß et al., 2014). Seeds suffer from winter mortality (50% mortality probability during winter) and die because of age (maximal age=1; i.e., there is no long-term seed bank simulated).

SEED DISPERSAL, GERMINATION AND ESTABLISHMENT

During the seed production period, plant individuals invest 5% of their acquired resources in the production of seeds (Schippers et al., 2001). In the following week of this period, all plants disperse their seeds. The direction is drawn from a uniform distribution and the dispersal distance depends on the PFT-specific seed characteristics and is drawn from a log-normal distribution (Stoyan and Wagner, 2001).

During the 2 seed establishment periods in the beginning of each simulated year (spring) and after seed dispersal (summer), seeds germinate with a probability of 50% (May et al., 2009; Körner et al., 2014; Weiß et al., 2014) and establish on ground (i.e., on cells that are not covered by any other individual). The chance of successful establishment depends on the seed mass, with heavier seeds assumed to be more competitive.

ABIOTIC FACTORS

In IBC-grass, resources (above- as well as below-ground) are distributed homogeneously in space and time. In addition, biotic disturbances such as grazing (selective removal of above-ground biomass), trampling (removal of individuals), and cutting (removal of above-ground biomass down to a certain height) are included. See the overview, design concepts, and details protocol in 7.2.1 for detailed information.

TEMPORAL DIMENSIONS

IBC-grass simulates the vegetation period of 30 wk per year (starting in spring, ending at the beginning of winter). As a result of environmental filtering and competition among PFTs, the PFT community is within a stable state after 150 yr. To avoid population and community level effects caused by this stabilization process, simulated herbicide application starts after another 25 yr (in year 175) and ends after 30 yr.

3.3.4 Implementation of herbicide-induced impacts

Herbicides potentially have an effect on the following plant attributes (according to the OECD, 2006a, 2006b; the US EPA, 2012a, 2012b, 2012c; Boutin et al., 2014): 1) Survival of plants: Implementation in IBC-grass: plants suffer from an additional herbicide-induced mortality probability. The strength of effect is determined by the specific effect intensity and is added after the density-dependent mortality. 2) Biomass of seedlings and plants: Implementation in IBC-grass: the biomass of seedlings and biomass gain of plants is reduced according to the specific effect intensity. 3) Establishment (emergence) of seedlings: Implementation in the IBC-grass model: the establishment probability of seedlings is reduced by the specific effect intensity. 4) Produced seed number: Implementation in the IBC-grass model: the resources available for seed production are reduced by the specific effect intensity. The PFT-specific seed weight is kept constant, resulting in a lower number of produced seeds. Finally, 5) Sterility of seeds: Implementation in IBC-grass: seed sterility is increased by adding an herbicide induced seed mortality probability according to the specific effect intensity that is comparable with seed fertility.

Herbicide application is simulated in the present theoretical parameters mentioned earlier (varying from 10–90% effect intensities). No underlying exposure assumptions of a specific herbicide application (e.g., over-spray, drift values, etc.) are considered. Herbicide application is simulated in the first week of each simulated year, bearing in mind that only the growing season starting in spring is simulated in IBC-grass (i.e., herbicide application takes place during spring). However, each of the herbicide-induced effects becomes effective only within the first week of the specific process. For example, seed production is simulated only in week 25; therefore, the herbicide effect on seed production occurs within this week 25. In this way, we were able to account for direct effects on each specific attribute. In addition, not only directly sprayed plants and seed individuals may suffer from an herbicidal effect (parental generation). Recently, concerns have been raised that sprayed plants might also pass on these effects to their offspring/seeds, resulting in effects on the F1 generation (generation carry-over effects; Boutin et al., 2014). Consequently, to address this concern in a conservative manner, we accounted not only for different attributes but also included generation carry-over effects. The timing of effects and the potentially affected individuals are summarized in Table 3.4.

Table 3.4: Overview of the timing and affected individuals for each attribute and affected generation

Attribute		Parental generation (P) Excl. generation carry over effects	Parental+F1 generation (P+F1) Incl. generation carry over effects
Mortality	Week of effect	1	1-3, 21-25
	Affected individuals	Existing plants in week 1	Existing plants in week 1 + F1 seedlings after their establishment in weeks 1-3 and 21-25
Biomass	Week of effect	4	4
	Affected individuals	Existing plants in week 1	Existing plants in week 4
Establishment	Week of effect	Week 1-3, 21-25	Week 1-3, 21-25
	Affected individuals	Existing seeds in week 1	Existing seeds in week 1 + produced seeds in week 19
Seed number	Week of effect	Week 19	Week 19
	Affected individuals	Existing plants in week 1	All existing plants
Seed sterility	Week of effect	Week 1	Week 1 or Week 20
	Affected individuals	Existing seeds in week 1	Existing seeds in week 1 + 20

3.3.5 Species-specific susceptibilities

To account for different species-specific herbicide susceptibilities, we tested dissimilar affected PFT groups. 1) All: All PFTs within the community are affected. This accounts for a broad spectrum herbicide (n=55). 2) Competitive: Only competitive PFTs that occur frequently (in more than 80% of the control Monte Carlo runs) in an isolated community are affected. This scenario was chosen to analyse the ecological sensitivity of the community and does not represent a realistic scenario. (Selectiveness of herbicides is mostly based on other trait characteristics of plants such as monocotyledonous versus dicotyledonous species) (n=4). 3) Less competitive: Only less competitive PFTs that occur frequently (in more than 80% of the control Monte Carlo runs) in an isolated community are affected. This scenario was used to analyse the ecological sensitivity of the community as a comparison with the competitive PFTs' scenario and probably does not represent a realistic case (n=4). 4) Monocotyledonous: Only monocotyledonous PFTs are affected. This scenario considers a selective herbicide acting only on monocotyledonous PFTs (n=14). 5) Dicotyledonous: Only dicotyledonous PFTs are affected. This scenario takes into account a selective herbicide acting only on dicotyledonous PFTs (n=40). The PFTs within these groups have the same susceptibility (1). Hence the effect intensity is equal for each of the affected PFTs. The distinction between monocotyledonous and dicotyledonous PFTs involves only the herbicide susceptibility (affected yes/no) and no other trait characteristics.

Table 3.5: Overview and explanation of study-specific terms

Term	Explanation
Effect intensity	Probability or rate of the individual level effect
Significant[a] effect intensity	Effect intensity which leads to a significanta effect extent
(Significant[a]) effect extent	Mean (relative) effect occurring at the population or community level (significant[a] if it is outside of the relative 2.5th and 97.5th control percentiles)
Mean significant[a] effect	Difference between the mean control percentiles (2.5th and 97.5th) and the mean significant[a] effect extent

[a] The term 'significant' in the context of this table does not refer to the concept of statistical significance

3.3.6 Scenarios

In addition to the different affected attributes (mortality, biomass, establishment, seed number, and seed sterility and the combination of mortality+biomass, mortality+biomass+seed number, and establishment+seed number+seed sterility), the generation (parental and parental+F1 [P and P+F1]), and the PFT group (all, competitive, less competitive, monocotyledonous, dicotyledonous), we also included 2 diverse seed input scenarios (isolated community without seed input [0 seeds/PFT/yr] and a community with moderate seed input [10 seeds/PFT/yr] and different effect intensities [from 10–90% effect intensity]).

3.3.7 Analyses

The output of the IBC-grass model is the population size per PFT per time step. Based on the population size, the inverse Simpson Diversity Index ($1/\Sigma p_i^2$ with p_i being the proportion of individuals belonging to species i) is calculated for each time step. The inverse Simpson Diversity Index was selected for analysis because it showed the strongest impacts in our scenarios compared with other diversity indices such as the Shannon-Wiener Index or evenness.

Each scenario includes 50 Monte Carlo runs (repeated 50 times) because of stochasticity and compared with control scenarios (also 50 Monte Carlo runs) in which no herbicide application is simulated. Each single Monte Carlo run is done in relation to the mean of the control (i.e., dividing by the mean of the control for both the population size and inverse Simpson Diversity Index). In a next step, the relative means for the treatment simulations and the 2.5th and 97.5th percentiles of the control simulations are calculated and again summarized over the entire herbicide application period of 30 yr (as a mean over 30 yr). If the treatment mean is outside the range of the means for the 2.5th and 97.5th percentiles of the control, a significant effect is assumed. Nevertheless, this type of significance should not be confused with statistical significance.

In this context, ecological sensitivity of a PFT community is the minimal effect intensity (see Table 3.5 for a definition) that is required to cause significant effects on the population size of 50% of the frequent (frequency > 0.8) PFTs or the minimal effect intensity that causes a significant effect of at least or more than 50% on the inverse Simpson Diversity Index. Ecological sensitivity of a PFT population level is the minimal effect intensity resulting in a mean significant effect extent. Smaller values show that the effect intensity that is applied to a specific PFT trait on the individual level to achieve significant effects is also small. Accordingly, smaller values represent a higher ecological sensitivity and thus a stronger impact on the PFT community and population.

If the analysis detects a significant effect, the mean significant effect was calculated (see Table 3.5 as an overview of study specific terms). This measure is the difference between the mean over the 30 yr of simulated herbicide application and the mean lower (or upper, depending on the effect direction [negative or positive]) percentile of the control. If the mean lower percentile (2.5th percentile) in the control is, for example, 0.7 (with 1.0 being the baseline) and the mean relative population size over this period in the treatment is 0.5, the mean significant effect would be –0.2 (–20%) but not –0.5 (–50%). In this way, the measure accounts for potential high variation within PFT population sizes in the control.

3.4 Results

3.4.1 Temporal behavior of the community

The temporal behavior of the simulated community is shown in Figures 3.2 and 3.3. In this exemplary scenario, the attributes seed number, seed sterility, and establishment are affected by 30% for the parental as well as the succeeding F1 generation (simulating a generation carry-over effect) in an isolated community (external seed input=0). Only dicotyledonous PFTs (n=41) are affected. Frequent dicotyledonous PFTs, marked with a

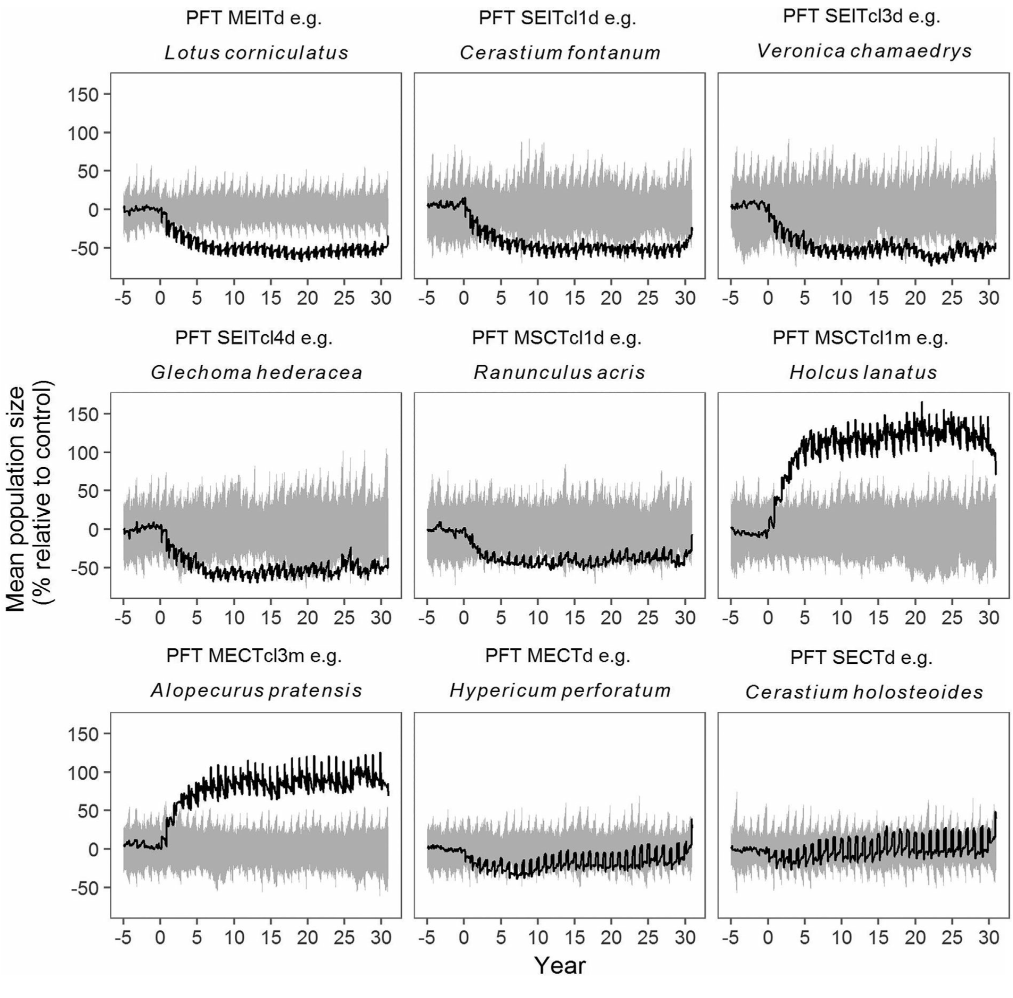

Figure 3.2: Effects of 30% effect intensity (per year) on seed number, seed sterility, and seed establishment on the population size of frequent plant functional types (PFTs) within an isolated community. Only dicotyledonous PFTs (PFTd) are affected. Black lines represent the mean in treatment relative to the mean of the control; gray ribbons show the variation within the control (in relation to the control mean). 5 yr before herbicide application (starting in year 0) and 30 yr of simulated herbicide application are displayed. The PFT ID is composed of the 4 trait syndromes: plant size (small [S], medium [M], and large [L]), growth form (erect [E], semi-rosette [S], and rosette [R]), resource response type (competitor [C], stress-tolerator [S], and intermediate [I]), and grazing response type (tolerator [T], avoider [A], and intermediate [I]); the clonal type (aclonal, short internodes with resource sharing [cl1], short internodes without resource sharing [cl2], long internodes with resource sharing [cl3], and long internodes without resource sharing [cl4]); and cotyledon characteristic (monocotyledonous [m] and dicotyledonous [d]).

"d" in Figure 3.2, show a strong decrease in population size. Nonetheless, the extent and temporal response are diverse. The PFTs MEITd (explanation of the PFT IDs can be found in the Materials and Methods section), representing (all plant species listed are examples) *Lotus corniculatus*, and SEIT, representing *Cerastium fontanum, Veronica chamaedrys*, and *Glechoma hederacea*, are strongly affected and show a long-lasting impact on population size over the simulated period. The PFT MSCTcl1d, representing *Ranunculus acris,* displays a lower but still long-lasting effect. In contrast, the PFTs MECTd (*Hypericum perforatum*) and SECTd (*Cerastium holosteoides*) indicate only short-term, negative effects. Both PFT populations are able to recover within a year and even reveal short-term increases in population size. The 2 frequent monocotyledonous PFTs MSCTcl1m (*Holcus lanatus*) and MECTcl3m (*Alopecurus pratensis*) display a strong, long-lasting increase in population size with high fluctuations within a year. Differences in the response of PFTs can be explained by the dissimilar trait characteristics (see Reeg et al., 2017 for a detailed discussion).

Looking at the entire community and diversity, a continuous decline in the inverse Simpson Diversity Index can be observed with short-term recovery during the second establishment period in autumn (Figure 3.3).

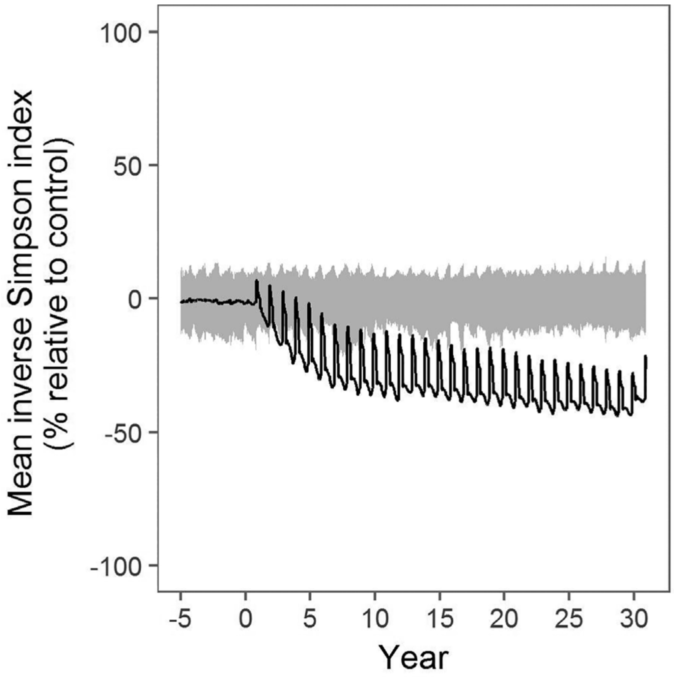

Figure 3.3: Effects of 30% effect intensity (per year) on seed number, seed sterility, and seed establishment on the inverse Simpson Diversity Index within an isolated community. Only dicots are affected. Black line indicates the mean in treatment relative to the mean of the control; gray ribbon identifies the variation within the control (in relation to the control mean). 5 yr before herbicide application (starting in year 0) and 30 yr of simulated herbicide application are shown.

3.4.2 Influence of the generation, the degree of isolation, the PFT group and the affected attribute

COMMUNITY LEVEL

In general, on a community level the inverse Simpson Diversity Index shows a strong decrease when both the parental and the F1 generation are affected (each attribute affected by 50%; Figure 3.4). An isolated (seed input=0) community indicates stronger effects than a community with external seed input (seed input=10). In the scenario where all PFTs are affected at the same intensity, the community displays the lowest negative response in the diversity index. Simulating herbicide-induced impacts which only act on frequent competitive PFTs (n=4), less competitive PFTs (n=4), or dicotyledonous PFTs (n=40) lead to strong negative effects on the diversity index. To summarize, strongest effects are found in an isolated community (seed input=0), when herbicide-induced impacts target only dicotyledonous species and also affect the F1 generation (P+F1).

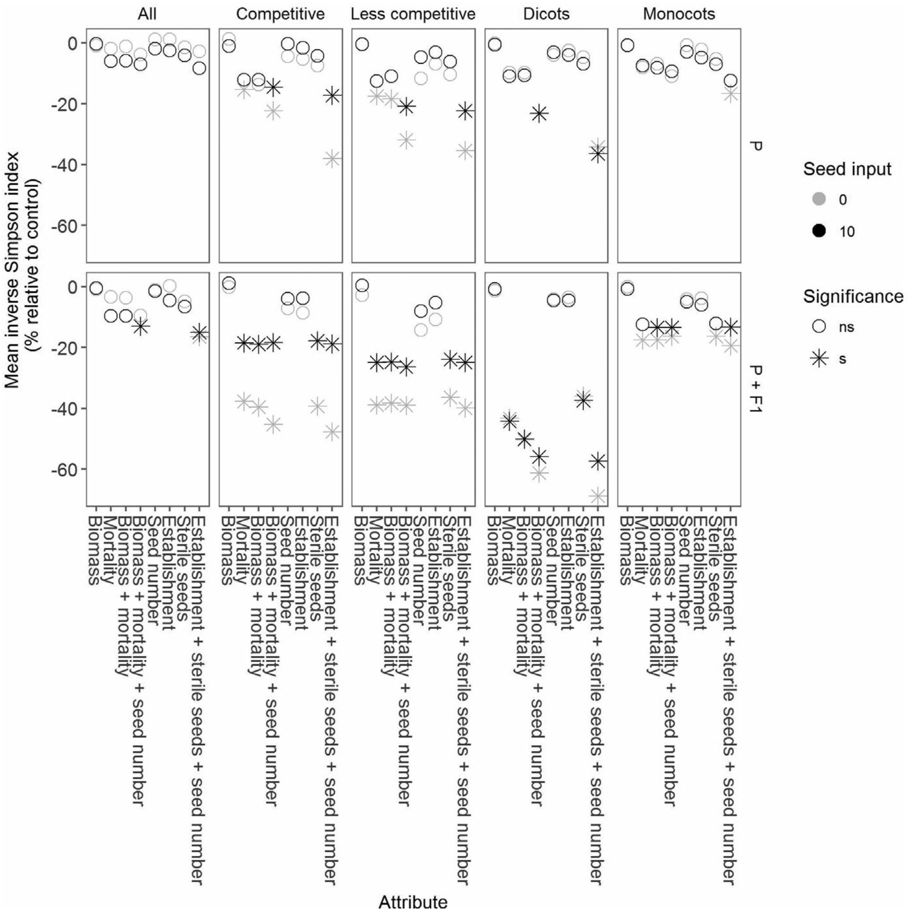

Figure 3.4: Effects of 50% reduction in each attribute on the inverse Simpson Diversity Index for different affected plant functional type (PFT) groups (all, competitive, less competitive, dicots, and monocots). Effects last for 1 wk. Inheritance of effects included in the P+F1 generations' scenarios (bottom row); no inheritance considered in the P generation scenarios (top row). Gray open circles denote isolated communities (0 seed input); black open circles include seed input of 10 seeds/PFT/year. Significant effects are marked with asterisks (condition for significance: mean of treatment is outside the range of control simulations).

Viewing the impacts on a community level for the single affected attributes, an increase in plants' mortality and in seed sterility reveal the strongest effect extents. A combination of affected attributes leads to stronger impacts on the inverse Simpson Diversity Index. The single effects of each attribute do not total in a linear fashion. For instance, in the worst-case scenario—where the parental and F1 generation of dicotyledonous PFTs are affected in an isolated community—a 50% effect intensity on the individual level only on biomass, or mortality, or seed number leads to a 2, 44, or 4% reduction of the inverse Simpson Diversity Index, respectively. A combination of these effects, that is, a 50% effect intensity on the individual level on each of these attributes at the same time, leads to a 61% decrease (slightly larger than the additive effects if only the single attributes are affected [2+44+4%, as mentioned above]). However, when only monocotyledonous PFTs are affected, a 50% effect on the single attributes already noted (biomass, mortality, and seed number) leads to 0, 17, and 4%, respectively. A combination on the other hand results in an even lower effect of only 16%.

POPULATION LEVEL

Now we focus on the scenario with the strongest effects (P+F1 generations are affected in an isolated community; seed input=0) as a very conservative scenario combining all the worst-case assumptions.

At the population level, direct negative as well as indirect positive effects are found (Figure 3.5). When all PFTs are affected by a 50% effect intensity, there are only a few PFTs displaying significant negative impacts on population size (all plant species listed are examples; for the single attributes: PFTs MEITd [*Lotus corniculatus*] and MECTd [*Hypericum perforatum*]; for the combined attributes: also PFT MECTcl3m [*Alopecurus pratensis*]). Only when the 3 reproductive attributes—establishment, seed sterility, and seed number—are affected in combination, PFT SEITcl1d (*Cerastium fontanum*) indicates a significant increase in population size. When only the frequent competitive PFTs are affected, a strong reduction in population size can be observed for these PFTs. Notwithstanding, there is also an indirect effect on the less competitive PFTs (assumed to be insensitive to the herbicide in this scenario), resulting in a strong enhancement of population sizes, especially when the attributes mortality and seed sterility are affected. The divergence between increase and decrease of population sizes is less pronounced when only the frequent less competitive PFTs are affected. However, the tendency is similar: population sizes of affected PFTs are decreased as a direct herbicide-induced effect and unaffected (insensitive) PFTs increase as an indirect effect. Thereby, the extent of the reduction and growth in population sizes is similar between PFTs of the same group (competitive/ less competitive). When all dicotyledonous PFTs are affected, their population sizes decrease to different extents depending on the PFT. The 2 monocotyledonous PFTs strongly increase in population size (as an indirect effect). Because there are only 2 monocotyledonous PFTs in the community, an herbicide induced population decline in these PFTs leads to a moderate boost in the population sizes of the dicotyledonous PFTs.

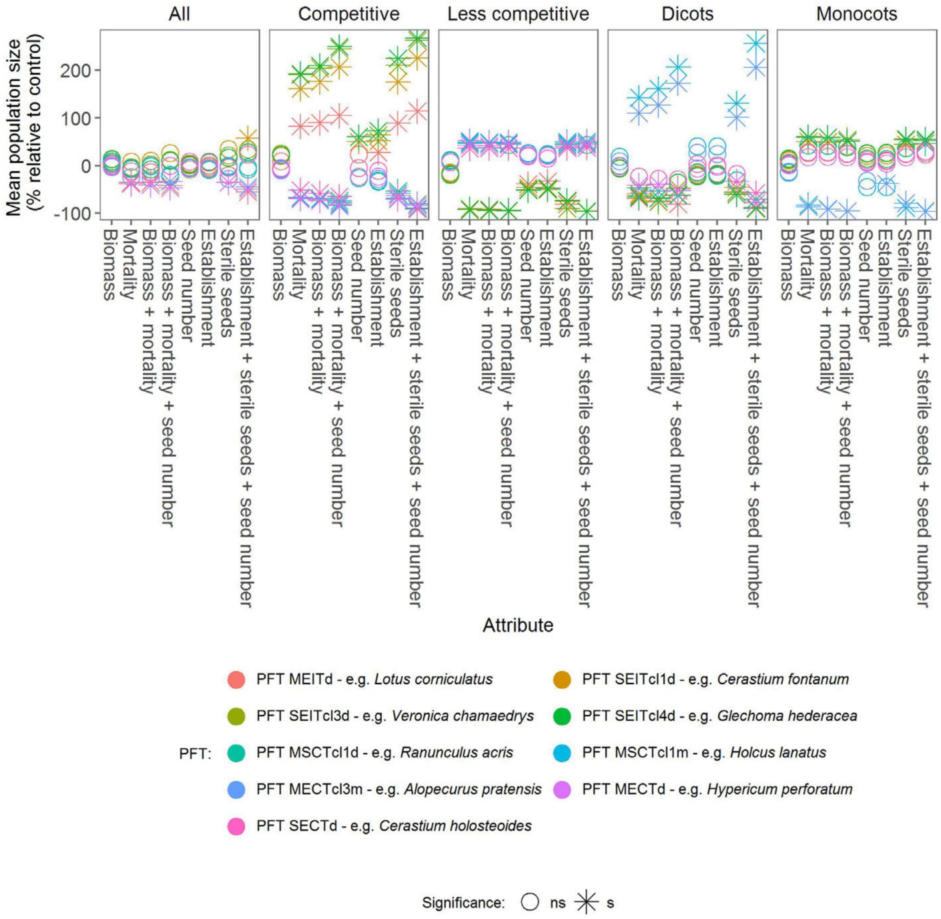

Figure 3.5: Effects of 50% reduction (effect intensity) in each attribute on the population sizes of all frequent plant functional types (PFTs) within an isolated community (seed input=0), whereas inheritance is included (P+F1). This theoretical worst-case scenario showed strongest effects on the community level. Significant effects are marked with asterisks (mean of treatment is outside the range of control). The PFT ID is composed of the 4 trait syndromes: plant size (small [S], medium [M], and large [L]), growth form (erect [E], semi-rosette [S], and rosette [R]), resource response type (competitor [C], stress-tolerator [S], and intermediate [I]), and grazing response type (tolerator [T], avoider [A], and intermediate [I]); the clonal type (aclonal, short internodes with resource sharing [cl1], short internodes without resource sharing [cl2], long internodes with resource sharing [cl3], and long internodes without resource sharing [cl4]); and cotyledon characteristic (monocotyledonous [m] and dicotyledonous [d]).

3.4.3 Ecological sensitivity analyses

In the present study, we describe the ecological sensitivity of a community (see Materials and Methods section for more information) to a potential herbicide as the effect intensity at which 50% of the PFT populations show a significant effect and/ or at which the inverse Simpson Diversity Index is decreased by more than 50% (Figure 3.6). The threshold of 50% was chosen to be comparable with median effect rate values that are the regulatory threshold for adverse effects in the European Union. In a global context, it should be considered that regulators may apply different effect thresholds or take additional safety factors into account. According to this definition, the scenario in which all PFTs have the same susceptibility shows the lowest ecological sensitivity because the PFT community is only affected under very high individual effect intensities. Only when the parental as well as the F1 generations are affected in the establishment of seedlings, the seed sterility, and the seed number in isolated communities, does an (unrealistically high) effect intensity of 60% lead to significant effects in 50% of the PFT populations. When only competitive PFTs are affected, the ecological sensitivity is much higher. Here, effect intensities as low as 20 to 30% lead to significant effects for at least 50% of the PFT populations. In this scenario, mortality and seed sterility are the ecologically most sensitive single attributes; that is, the effect intensities leading to significant impacts on at least one-half of the PFT populations are lowest for these attributes compared with the other tested attributes. A combination of 3 attributes (biomass, mortality, and seed number, as well as establishment, seed sterility, and seed number) shows even higher impacts on the PFT community. Including seed input as a means of increasing realism reduces the impact. When less competitive or monocotyledonous PFTs are affected, moderate seed input even erases the ecological impact; that is, there is no significant effect on more than one-half of the PFT populations.

The inverse Simpson Diversity Index displayed the highest ecological sensitivity in the scenario where dicotyledonous PFTs are affected. Here, effect intensities of more than 40% reveal a significant reduction in the diversity index of more than 50% when all reproductive attributes are affected (50% each effect on establishment, seed sterility, and seed number). Thus the highest impacts on the PFT community occur when only dicotyledonous PFTs are targeted.

Furthermore,we were also interested in the effect intensities at which the population size and the diversity index showed significant impacts (Figure 3.7). In this context, ecological sensitivity of a PFT population is the effect intensity at which significant impacts occur: the lower the value the higher the sensitivity. To illustrate,we selected a conservative but still realistic scenario: the parental and the F1generations are affected, the local community has a moderate seed input (10 seeds/yr/PFT), and the herbicide targets all, dicotyledonous, or monocotyledonous PFTs.

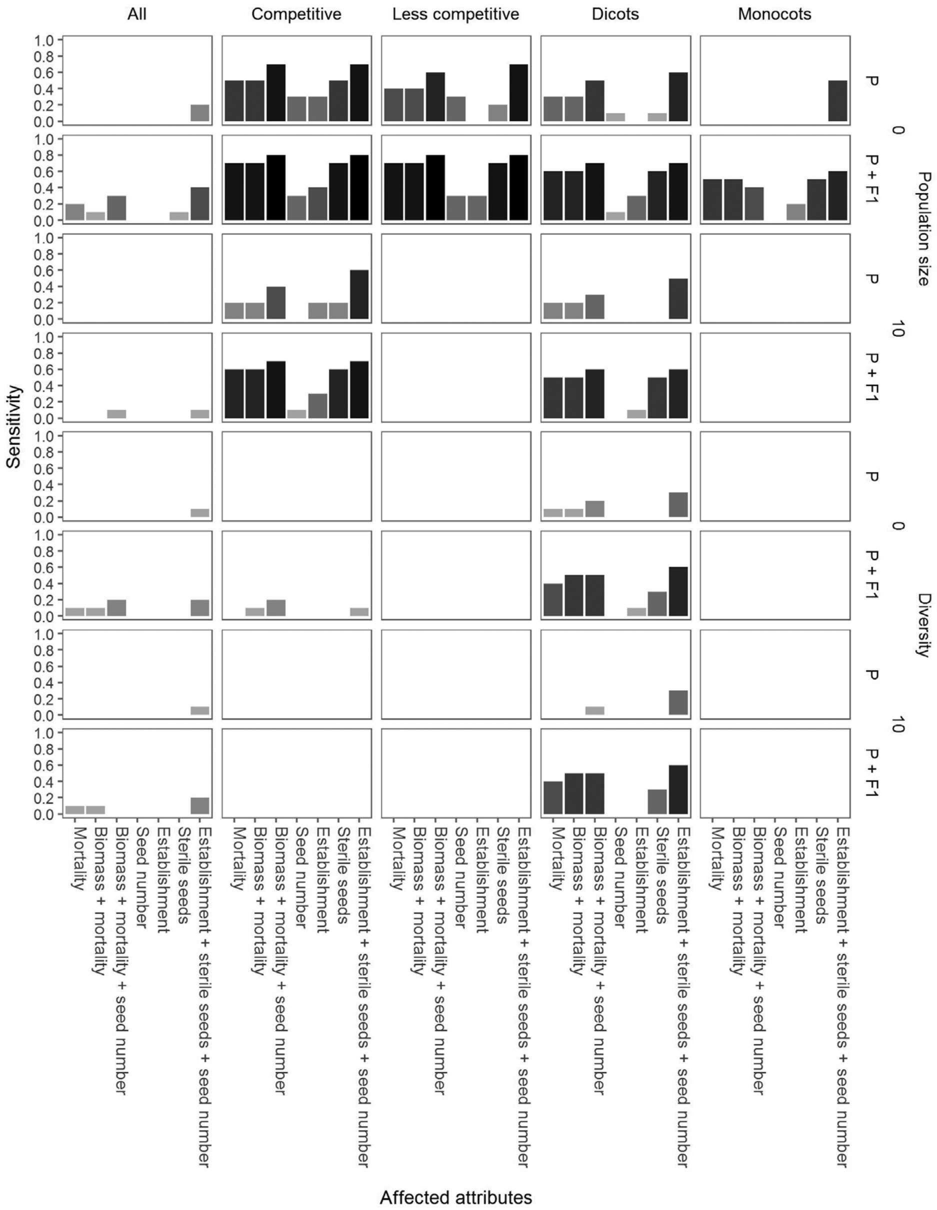

Figure 3.6: Ecological sensitivity of attributes/attribute combinations for different affected plant functional type (PFT) groups (all, competitive, less competitive, dicots, and monocots), diverse degrees of isolation (no external seed input [0] and 10 seeds/PFT/year [10]), and contrasting affected generations (P—no inheritance to seeds; P+F1—inheritance included) based on population size and the inverse Simpson Diversity Index as ameasure of diversity. Ecological sensitivity is definedas theminimal significant effect intensity atwhich 50%of the frequent (frequency>0.8) PFT populations display a significant effect on population size or the inverse Simpson Diversity Index indicates a significant effect of at least 50%. For better visualization, the minimal significant effect intensity is subtracted from one (i.e., 60% effect intensity is shown as 0.4). Thus the higher the bar, the greater the sensitivity.

When all PFTs are targeted, the PFTs MECTd (all plant species referred to are examples; *Hypericum perforatum*) and MEITd (*Lotus corniculatus*) are ecologically most sensitive; significant effect extents occur at the lowest effect intensities compared with the other PFT populations, when the combination of reproductive attributes (establishment, seed sterility, and seed number) is affected. An effect intensity of 40% on each attribute leads to the first significant effect extents for these PFTs. However, the mean significant effects (% decrease or increase below or above the 2.5th or 97.5th percentile of the control; see Materials and Methods section for more information) are only a 4%(PFT MEITd, *Lotus corniculatus*) and a 0.2% (PFT MECTd, *Hypericum perforatum*) decrease. For this attribute combination, the population sizes of the other PFTs indicate a significant effect only at 50 to 90%effect intensity with a mean significant effect of – 42% (decrease) through 7% (increase). For the other 2 attribute combinations (biomass and mortality; biomass, mortality, and seed number) and the single attribute of mortality, the lowest significant effect intensity was between 50 to 90% with mean significant effect extents of –21% (decrease) through 11% (increase). The PFTs SECTd (*Cerastium holosteoides*), MECTd (*Hypericum perforatum*), MECTcl3m (*Alopecurus pratensis*), SEITcl1 (*Cerastium fontanum*), and MEITd (*Lotus corniculatus*) display significant impacts on population level at an effect intensity of 50 to 90% on the attribute of seed sterility with negative mean significant effects of up to 13%. For all PFTs, an effect on the seed number and the establishment does not have significant impacts up to an effect intensity of 80%.

When only dicotyledonous PFTs are affected, population sizes of both monocotyledonous PFTs MECTcl3m (*Alopecurus pratensis*) and MSCTcl1m (*Holcus lanatus*) increase significantly when the single attribute of mortality or the attribute combinations of biomass and mortality; biomass, mortality, and seed number; or establishment, seed sterility, and seed number are affected by 20% each. The highest mean significant effects occur within the 3-fold combinations and lead to a mean increase of 17 to 25% (above the 97th percentile of control simulations). In this scenario, the ecologically most sensitive single affected attribute for dicotyledonous PFTs is mortality, closely followed by seed sterility. Individual level effect intensities resulting in significant impacts at the population level vary from 30 to 50% depending on the PFT. The ecologically most sensitive PFT is MEITd (*Lotus corniculatus*) with a negative significant effect extent of 13% at 30% effect intensity on mortality. At the same effect intensity, significant effects occur for seed sterility. However, the negative significant effect extent is only 5%. The combination of affected attributes increases the ecological sensitivity slightly. For the combination of effects on establishment, seed sterility, and seed number, all PFTs show the first significant effects at effect intensities

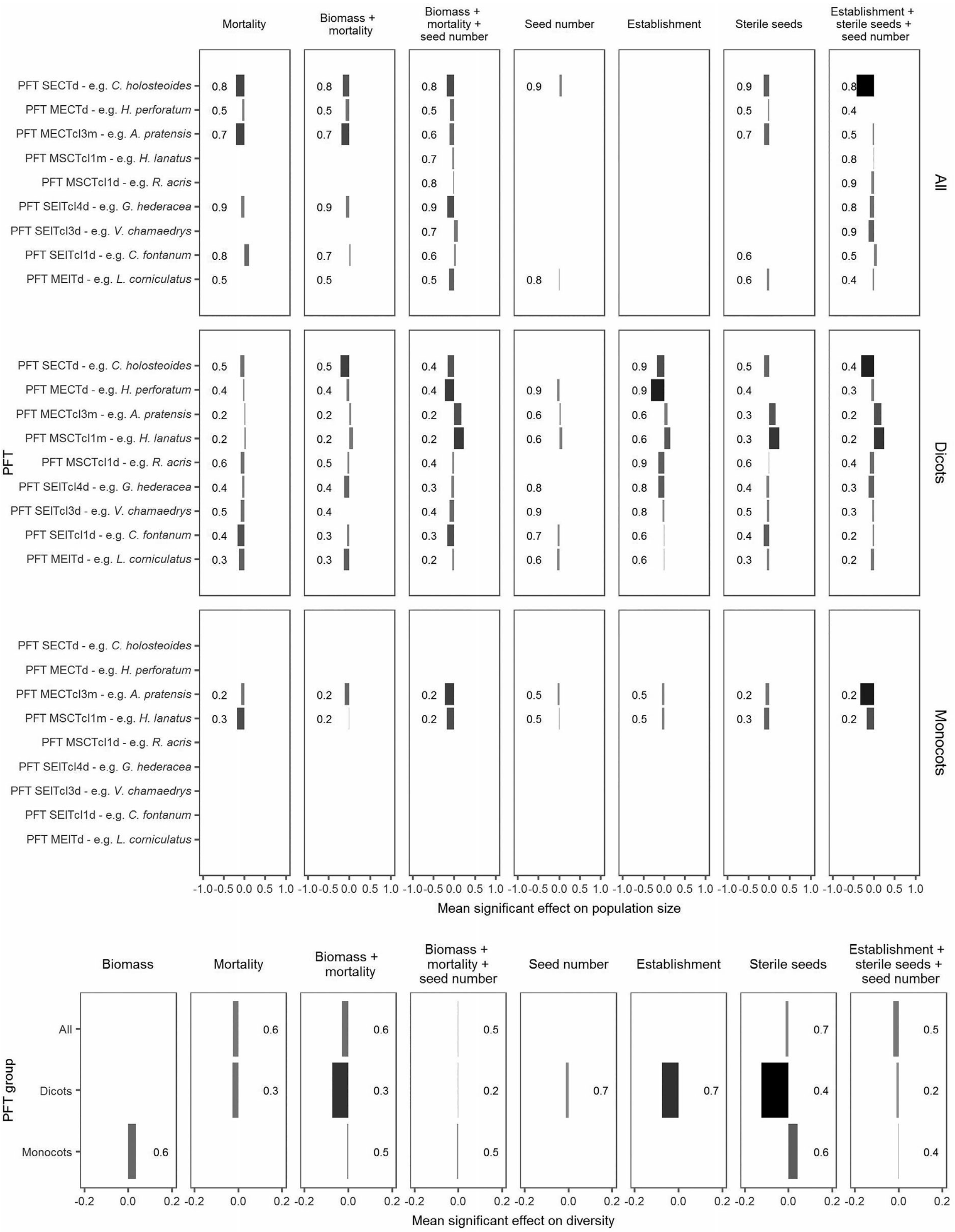

Figure 3.7: Mean significant effect extent on each plant functional type (PFT) population (3 top rows, effects on population size) and the community (bottom row, effects on inverse Simpson Diversity Index). Numbers show the minimal effect intensity resulting in a mean significant effect extent illustrated by the height of the bars. The lower the numbers, the higher the sensitivity of the PFT. The image indicates only the more realistic scenarios with seed input (10 seeds), where both generations P and F1 are affected (inheritance is included). The PFT ID is composed of the 4 trait syndromes: plant size (small [S], medium [M], and large [L]), growth form (erect [E], semi-rosette [S], and rosette [R]), resource response type (competitor [C], stresstolerator [S], and intermediate [I]), and grazing response type (tolerator [T], avoider [A], and intermediate [I]); the clonal type (aclonal, short internodes with resource sharing [cl1], short internodes without resource sharing [cl2], long internodes with resource sharing [cl3], and long internodes without resource sharing [cl4]); and cotyledon characteristic (monocotyledonous [m] and dicotyledonous [d]).

of 20 to 40%. Plant functional types SEITcl1d (*Cerastium fontanum*) and MEITd (*Lotus corniculatus*) have the highest ecological sensitivity. Nevertheless, the mean significant effect extents are 4 and 8%, respectively. On the other hand, PFT SECTd (*Cerastium holosteoides*) shows the lowest ecological sensitivity of 40% effect intensity but exhibits a high mean significant effect extent of 32%. The 3-fold combination of biomass, mortality, and seed number displays a slightly lower ecological sensitivity for most dicotyledonous PFTs with either higher effect intensities or lower effect extents at the same intensity level. The single attributes of seed number and establishment indicate low ecological sensitivities only at effect intensities of 60 to 90%.

When monocotyledonous PFTs are targeted, there are no significant (indirect) effects for dicotyledonous PFTs. However, the 2 frequent monocotyledonous PFTs are quite sensitive to effects on all single attributes and attribute combinations (i.e., there are significant effects at effect intensities of 20–30%), except for the single attributes of seed number and establishment (significant effects at effect intensities of 50%).

The inverse Simpson Diversity Index is ecologically most sensitive in the scenario where dicotyledonous PFTs are targeted; in other words, there is a high impact on the diversity already at low effect intensities. Especially if a 3-fold combination of affected attributes is considered, the inverse Simpson Diversity Index shows strong impacts. At effect intensities of 20% on each of the attributes, the index shows a mean significant decrease of 0.2% (biomass, mortality, and seed number) through 2% (establishment, seed sterility, and seed number).

3.5 Discussion

Reproductive performance is an important factor for plant population and community dynamics. However, the toxicological sensitivity of plants to reproductive impairment is not well characterized and current standard ecotoxicological tests (OECD, 2006a, 2006b; USEPA, 2012a, 2012b) do not directly address reproductive endpoints such as seed production. To address the uncertainty associated with reproductive endpoint sensitivity in the ecotoxicological tests, we adapted the individual-based plant community model for grasslands (IBC-grass) to compare the consequences of herbicide- induced effects on vegetative endpoints (biomass and plant mortality) with effects on reproductive endpoints (seed sterility, seed establishment, and seed production) at the population and community level. Because we were interested in a general understanding of potential differences between vegetative and reproductive endpoints, we systematically varied herbicide effects by a variable, randomly chosen percentage of reduction of plant biomass or survival in comparison with reduced reproduction parameters rather than focusing on specific exposure patterns related to actual herbicidal products.

Seed sterility (ability of seeds to germinate) and plant mortality were the ecologically most sensitive attributes in the present study, showing significant impacts on population and community levels already at low effect intensities. An herbicide induced increase in seed sterility or plant mortality even at low effect intensities (individual level effect on the specific attribute) resulted in the highest impacts on the PFT populations and the PFT community. Indeed, both attributes are included as endpoints in the current OECD and USEPA guidelines, where effects on the survival of plants and the emergence of seedlings after exposure to a plant protection product are measured (OECD, 2006a, 2006b; USEPA, 2012a, 2012b). In contrast to the consequences of effects on seed sterility and plant mortality on population and community levels, a reduction in seed production (lower number of produced seeds), establishment probability, or biomass had negative impacts on PFT populations and the community only under very high herbicidal effect intensities (i.e., high percentage reduction of the specific endpoint).

Several experimental studies have analysed herbicide effects on reproductive attributes (Strandberg et al., 2012; Boutin et al., 2014; Schmitz et al., 2014). In contrast to our findings, Strandberg et al. (2012) concluded that seed production was a more sensitive (from the toxicological perspective) endpoint than biomass for some of the tested species. Nonetheless, the present study focuses on long-term population and community level effects, whereas Strandberg et al. (2012) investigated short-term effects at the individual level. Supporting our findings, Boutin et al. (2014) and Rotchés-Ribalta et al. (2015) found that the individual level sensitivity of reproductive endpoints relative to vegetative endpoints is species dependent.

There are only a few experimental (and no modelling) studies focusing on long-term effects (e.g., 3-yr study of Schmitz et al. 2014), which are considered particularly important to addressing the specific protection goals for non-target terrestrial plants (EFSA PPR Panel, 2010). Schmitz et al. (2014) could detect seed reduction and flower suppression for 3 out of 4 tested species after application of an herbicide at 30% of the field application rate. Even though the application rate far exceeds the expected off-field exposure rate under worst-case conditions, they were not able to observe an impact at the plant community level. It is necessary to show not only short-term, individual level effects but also to investigate long-term effects on the population and community. The comparison of the available experimental studies with our results clearly indicates that the IBC-grass model is a valuable tool for reducing the uncertainty associated with extrapolating conclusions from the short-term, individual level effects to the long-term, population level and community level effects.

Assuming the occurrence of generation carry-over effects, in which case the F1 generation of a sprayed individual is still affected (e.g., emergence of seedlings is impacted in the P and F1 generations), the ecological sensitivity of each endpoint increased and significant impacts were detectable at lower effect intensities (see Figure 3.6). A sophisticated modelling approach based on the IBC-grass model, which includes realistic herbicide impacts as measured in the standard non-target plant guideline studies (see Reeg et al., 2017) and in addition integrates potential generation carry-over effects, could represent a good option to estimate potential ecological risks. Such an approach has the advantage of analysing various potential scenarios—in this case various scenarios of generation carry-over effects. In the event that the mode of action indicates potential generation carry-over effects, an IBC-grass based higher tier evaluation might support the assessment of long-term risks to non-target terrestrial plants. For the presented modelling exercise, it should be kept in mind that the inclusion of effects on the next generation (especially to the extent investigated for the present study) is based on theoretical, worst-case assumptions that are not derived from actual experience and observation of such effects.

In summary, the current OECD and USEPA guidelines cover the ecologically most sensitive endpoints for protection of plant populations and communities—seed sterility and plant mortality. Seed production does not necessarily need to be investigated, as long as there is no indication that the herbicide has very strong effects at the individual plant level (>50%) in off-field areas. Considering the fact that seed dormancy and thus long-term seed banks (i.e., viable seeds within the soil) are not included in the current IBC-grass version, our model results are quite conservative. Long- as well as short-term seed banks can serve as buffer mechanisms for disturbances such as herbicide impacts. Reductions in seed production can be balanced by a seed bank from which seeds can establish, or locally extinct plant species are able to recolonize (Bakker et al., 1996). Thus, if at all, including a seed bank in our model would have led to lower effects than those shown.

3.6 Conclusions

The extensive sensitivity analyses of potentially affected plant attributes at the individual level and the resulting long-term impact at the population and community level provide great insights into the current debate on the individual level sensitivity of reproductive versus vegetative endpoints and their consequences for plant communities in ecological risk assessment. The present study underlines the importance and the potential of modelling studies in risk assessments as a tool to indicate and predict ecologically relevant impacts of herbicides on non-target terrestrial plant communities. At the same time, suitable empirical studies on a community level are needed to validate the model and thereby confirm and strengthen the model results. Validated community level modelling studies can support regulators in their decisions about the appropriate risk assessment endpoints and provide confidence in their assessments.

4 Modelling direct and indirect effects of herbicides on non-target grassland communities[1]

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[1] published as: Reeg J, Schad T Preuss TG, Solga A, Körner K, Mihan C, Jeltsch F. 2017. Modelling direct and indirect effects of herbicides on non-target grassland communities. Ecological Modelling. 348: 44-55. DOI: 10.1016/j.ecolmodel.2017.01.010

4.1 Abstract

Natural grassland communities are threatened by a variety of factors, such as climate change and increasing land use by mankind. The use of plant protection products (synthetic or organic) is mandatory in agricultural food production. To avoid adverse effects on natural grasslands within agricultural areas, synthetic plant protection products are strictly regulated in Europe. However, effects of herbicides on non-target terrestrial plants are primarily studied on the level of individual plants neglecting interactions between species.

In our study, we aim to extrapolate individual-level effects to the population and community level by adapting an existing spatio-temporal, individual-based plant community model (IBC-grass). We analyse the effects of herbicide exposure for three different grassland communities: 1) representative field boundary community, 2) *Calthion* grassland community, and 3) *Arrhenatheretalia* grassland community. Our simulations show that herbicide depositions can have effects on non-target plant communities resulting from direct and indirect effects on population level. The effect extent depends not only on the distance to the field, but also on the specific plant community, its disturbance regime (cutting frequency, trampling and grazing intensity) and resource level.

Mechanistic modelling approaches such as IBC-grass present a promising novel approach in transfer-ring and extrapolating standardized pot experiments to community level and thereby bridging the gap between ecotoxicological testing (e.g. in the greenhouse) and protection goals referring to real world conditions.

4.2 Introduction

Worldwide, the use of herbicides on conventionally managed arable fields is common practice for controlling weeds and safe-guarding yields (Ecobichon, 2001; van der Werf, 1996; Wilson and Tisdell, 2001). Depending on wind conditions and application methods it is almost inevitable that small amounts of these herbicides spread into habitats in the vicinity of agricultural fields (field boundaries), i.e. non-target areas (de Snoo and van der Poll, 1999). Spray drift is largely driven by spatial and temporal variability of environmental, ecological and agricultural conditions, e.g. the composition and structure of the landscape, weather events, spray-drift variability and application technology. Since herbicides are developed to control specific plant species considered as harmful within an agricultural field, i.e. weeds, and have lethal effects on those tar-get species, plant individuals occurring in field boundaries have a potentially high risk to be affected in a similar way when exposed to deposits (de Snoo and van der Poll, 1999; Kleijn and Snoeijing, 1997; Kleijn and Verbeek, 2000; Marrs et al., 1993). To mitigate exposure of those communities, measures like the use of drift reducing spray nozzles or consideration of buffer zones are regularly applied. However, such measures cannot always fully eliminate drift exposure.

Field boundaries are quite diverse. They include herbaceous field margins like ditches or river banks as well as hedges or forest edges. In some cases, meadows and grasslands are located in immediate proximity. Due to the use of fertilizers and management activities, field boundaries are characterized by a medium to high nutrient availability and disturbances such as trampling and mowing. Grassland communities are crucial for maintaining biodiversity within European landscapes. Natural grassland communities are threatened by climate change and increasing land use. Food and energy production by agriculture reduces the area available for semi-natural grassland communities. The use of plant protection products (synthetic or organic) is mandatory in agricultural food production. To avoid adverse effects on natural grassland communities within the agricultural areas strict regulations for synthetic plant protection products are in place in Europe and environmental risk assessments are conducted. The basis of these risk assessments are standardized biotests conducted at individual-level in the lab-oratory (e.g. OECD guideline studies (OECD, 2006a, 2006b)). In contrast to the level of individual plants, the European Food and Safety Authority (EFSA) developed specific protection goals towards the protection on population and community level (EFSA PPR Panel, 2014). Specific protection goals for non-target terrestrial plants are primary production, nutrient cycling, water regulation, provision of habitat and food, among others. These goals can be met by protecting populations, functional groups, and/or communities considering diversity, population abundances, and/or biomass. Therefore, cur-rent individual-level OECD guidelines seem not to be sufficient to address these specific protection goals.

The scientific community has largely neglected to study species interactions, historically measuring the effects of herbicides on individual plants rather than communities (Dalton and Boutin, 2010). The number of existing experimental studies on the level of plant communities (de Snoo and van der Poll, 1999; Kleijn and Snoeijing, 1997; Marrs et al., 1993; Schmitz et al., 2014) is small which can mainly be attributed to the complexity of those trials with regard to variability, labour, and costs. Although duration of these community experiments available from the literature was up to three years, from the perspective of vegetation analysis the study periods were rather short. While longer experiments may provide new insights in plant community dynamics impacted by chemical stressors, the complexity of community-level experiments as well as the needed time and resources make it unlikely that empirical long term studies will be available in the future. Therefore, mechanistic computer models can provide an alternative approach to better understand non-target community effects. These mechanistic modelling approaches should be designed in a way that the available knowledge can be integrated and, hence, community interactions emerging from the models can be validated and tested. As stated above, most studies investigate the effects of herbicides on single plant species. In addition, competition of plant species depends on the direct neighbourhood. Therefore, the model approach should be individual-based and spatially explicit.

In our study, we adapt an existing spatio-temporal, individual-based plant community model (IBC-grass, Körner et al., 2014; May et al., 2009; Weiß et al., 2014) to analyse population and community level effects of herbicide exposure for grassland communities. IBC-grass simulates herbaceous plant community patterns on a local scale (patch of approx. 3 m^2) by taking below- and aboveground interactions between individuals into account. To explore realistic herbicide effects at the individual-level we add a toxicological submodel to IBC-grass. The effect rate on the simulated vegetation patch is gained from a species effect distribution calculated by the exposure model Xplicit (Schad and Schulz, 2011; Schad, 2013). Xplicit simulates herbicide exposure in field boundaries and calculates effect rates on plant individual-level depending on the specific spatial location of the patch in the landscape as well as on the ecotoxicological standard tests used for environmental risk assessment of herbicides in Europe (OECD, 2006a, 2006b).We simulate the effect of herbicide exposures to three different plant communities: 1) a representative field boundary community, 2) a *Calthion* grassland community and 3) an *Arrhenatheretalia* grassland community. The communities differ in their regional species pool, management regime and resource level, which are determining factors for the composition and dynamics of grassland communities. We expect that (i) herbicide exposure will influence the interactions and resource competition between plant individuals and therefore cause direct and indirect effects on population and community level, and (ii) community response to herbicide exposure will depend on the specific species pool, management regime and resource level. For each community, we simulate local community patches at different distances to the treated arable field to account for effects of buffer zones as a potential mitigation measure.

4.3 Methods

4.3.1 Plant communities

A representative 'field boundary community' is based on a recent literature review on species found in such habitats in Europe (Kolja Bergholz unpublished, see 7.3.1, Table 7.8 for species list). In addition, we include two grassland communities with different management regimes and nutrient levels, which are common in Central Europe: (i) *Calthion*, which is a plant community that occurs in wet meadows with medium nutrient availability and (ii) a representative *Arrhenatheretalia* community that occurs in fertile meadows often used as pastures with high nutrient availability. To assess the species pool of those communities we reviewed vegetation surveys by Dierschke and colleagues (Dierschke, 2004; Dierschke et al., 2004; Fischer, 1985) and included expert knowledge (Michael Ristow, personal communication, see 7.3.1, Tables 7.9 and 7.10 for species lists). The environmental conditions for these two communities differ in their nutrient availability and the amount of cutting events per year (Table 4.1).

Table 4.1: Summary of abiotic parameters of simulated plant communities. Field boundary represents a community based on a literature review by Kolja Bergholz; Arrhenatheretalia represents a grassland community with high disturbances by trampling and Calthion a meadow with few disturbance events to account for different disturbance intensities.

	Field boundary	*Arrhenatheretalia*	*Calthion*
Belowground resources	high	high	medium
Disturbances			
Cutting per year [at 500mg dw/cm^2]	1	3	1
Trampling [% area/year]	10%	10%	2%

4.3.2 The IBC-grass model

Plant community dynamics are driven by abiotic as well as biotic factors. Environmental characteristics such as nutrient levels, light and disturbances by either agricultural managements (e.g. by tractor crossings) or herbivory (e.g. grazing and trampling) determine the abiotic conditions in the community. Over time, plant individuals compete for resources and space. Thereby, the specific trait characteristics of a plant individual determine the growth potential and competitive strength.

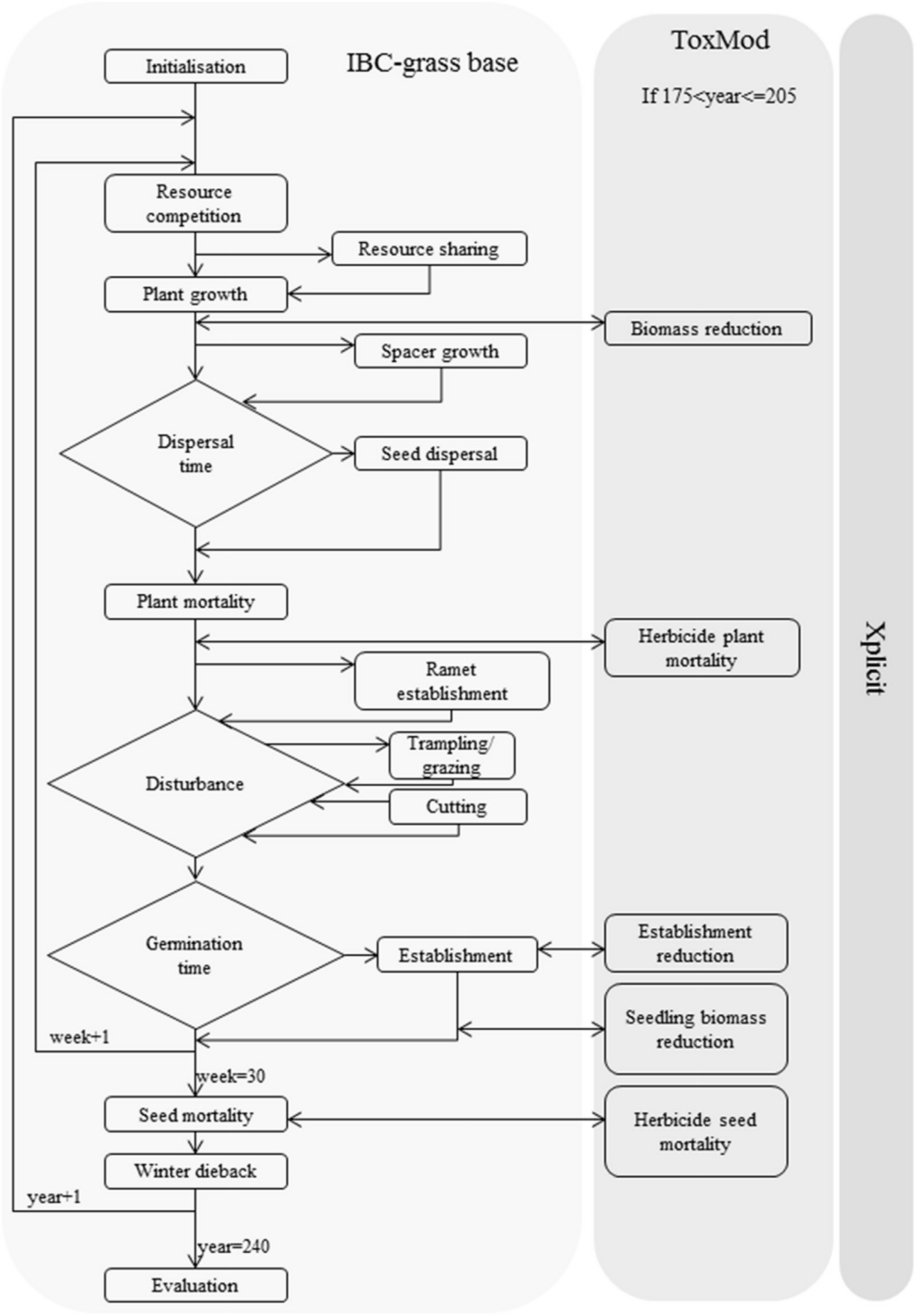

Figure 4.1: Flowchart and graphical illustration of IBC-grass. Chronology of the different processes within IBC-grass is displayed. A detailed description of each process can be found in 7.3.2.

IBC-grass is a well-established plant community model, which simulates local dynamics taking into account those main drivers. We base our approach on the published IBC-grass model of Weiß et al. (2014) enhancing it by adding an herbicide effect module and improving existing submodels. The flowchart (Figure 4.1) gives a general overview of the considered processes in IBC-grass, main state variables can be found in Table 4.2. A detailed description of the base model and our modifications following the ODD protocol (Grimm et al., 2006, 2010) including all state variables and equations can be found in 7.3.2. In the following we give a summary of the main aspects, approaches and modifications in IBC-grass.

Table 4.2: Main state variables of IBC-grass including a short explanation and the unit. More details can be found in the methods and ODD protocol in 7.3.2.

Variables	Explanation	Unit
type	PFT ID	
x_{coord}, y_{coord}	location of the plant‘s stem on the grid	
age	age of the plant	years
$m_{shoot/root/repro}$	shoot/root/reproductive mass	mg
w_{stress}	consecutive weeks of stress (i.e. lack of resources)	weeks
SpacerLength	current spacer length	cm
Spacerdirection	spacer direction	
$Res_{A/B}$	Above- and belowground resources per cm^2	Resource units

TRAIT-BASED APPROACH

IBC-grass makes use of a trait-based approach, which classifies species into plant functional types (PFTs) according to their specific trait characteristics (Table 4.3), i.e. one PFT represents one or several plant species, which can be expected to respond in a similar way to abiotic and biotic conditions, e.g. resource competition, grazing intensities. Thus, general processes in grassland communities are captured whilst being transferable and general enough to allow conclusions for several grassland communities.

Overall, six different trait syndromes are considered in the standard IBC-grass model (Table 4.3). All plant species of the regional species pool (see 7.3.2) are parameterized using the trait data bases BiolFlor, LEDA and cloPla3 (Kleyer et al., 2008; Klimešová and de Bello, 2009; Klotz et al., 2002, see also Table 4.3). Thereby, each plant species can be classified into a PFT. An overview of the plant species and their classification to PFTs can be found in Tables 7.8–7.10 in 7.3.2.

Table 4.3: Trait syndromes, PFT specific trait parameter values and used databases.

Trait/trait syndrome and attributes	Trait parameters				Database
Growth form	f_{leaf}				BiolFlor- rosette attribute
Rosette	1				rosette
Intermediate	0.75				Semi-rosette
Erect	0.5				erect
Maximum plant size	m_{max}	m_{seed}	$mean_{disp}$	std_{disp}	LEDA - seed releasing height
Large	5000 mg	1 mg	0.1 m	0.1 m	>0.87m
Medium	2000 mg	0.3 mg	0.3 m	0.3 m	0.42-0.87m
Small	1000 mg	0.1 mg	0.6 m	0.6 m	<0.42m
Resource response	ru_{max}	$surv_{max}$			BiolFlor - plant strategy type
Competitor	60 resource units	2 weeks			c, cr
Intermediate	40 resource units	4 weeks			csr, r
Stress-tolerator	20 resource units	6 weeks			sr, cs, s
Grazing response	palat	c_{shoot}			BiolFlor – indicator values grazing tolerance
Tolerator	1	1			4-6
Intermediate	0.5	0.75			1-3
Avoider	0.25	0.5			7-9
Herbicide susceptibility	Sens				Randomly distributed
	0-1				
Clonal integration	Resshare				cloPla3 – persistence of connection
Integrator	1				>=2 years
Splitter	0				<2 years
Lateral spread	SpacerL	stdSpacerL			cloPla3 – lateral spread
Short	2.5 cm	2.5 cm			<0.01 m/y
Long	17.5 cm	12.5 cm			0.01-0.25 m/y and longer

SPATIAL DIMENSIONS

IBC-grass simulates plant community dynamics on a local patch of approx. 3 m^2. The local patch is divided by 173 × 173 grid cells of 1 cm^2 each. Periodic boundary conditions are used to avoid edge effects. Two layers are distinguished in IBC-grass: aboveground and belowground.

Each grid cell can fit the stem of one plant. The position of a plant's stem is defined by the state variables x_{coord} and y_{coord}. In an aboveground and in a belowground layer the plants' roots and shoots cover a circular area around its stem ($A_{shoot/root}$, Table 4.4) ('Zone-of-Influence' (ZOI)). The above and belowground ZOIs are determined by the specific root and shoot mass ($m_{shoot/root}$), root and shoot geometry ($c_{shoot/root}$), and the growth form of the plant individual ($f_{leaf/root}$). ZOIs of neighbouring plant individuals can overlap. Within these overlapping zones, plants compete for light (aboveground) and belowground resources (see Section *Interactions and growth*).

In contrast to established plants, several seeds can be located in one grid cell. Like with plants, the location of a seed is stored by their x and y coordinates (x_{coord}, y_{coord}). Seeds can only germinate and establish if the cell is not covered by the aboveground ZOI of any other plant individual. Seed dispersal distance is dependent on seed mass, and drawn from a log-normal and the direction from a uniform distribution (Stoyan and Wagner, 2001).

INTERACTIONS AND GROWTH

Each plant is defined by its current size, neighbourhood, and specific trait characteristics, such as competitive strength and growth potential. Plant individuals compete for resources within the over-lapping regions of their ZOI (Table 4.4). Aboveground, asymmetric competition is simulated such that taller individuals (as resulting from their current aboveground biomass and their growth form) will acquire more light than smaller individuals (Table 4.4). Plant growth depends on the constant conversion rate g of resources into biomass, the acquired resources *res*, the current shoot mass and the specific trait characteristics of the shoot c_{shoot}, growth form f_{leaf}, maximal resource utilization ru_{max}, and the maximal plant mass m_{max}. In the absence of competition, plants show a sigmoid growth (Table 4.4, Eq. 'shoot/root growth', see also in Berger et al., 2008; DeAngelis and

Table 4.4: Main equations in IBC-grass regarding competition, growth and mortality. More details can be found in the methods and ODD protocol.

Process	Equation	Variables
Zone of influence (ZOI)	$A_{shoot} = c_{shoot} * (f_{leaf} * m_{shoot})^{2/3}$ $A_{root} = RAR * m_{root}^{2/3}$	c_{shoot} – PFT specific leaf area RAR – root form (1) f_{leaf} – PFT specific growth form
Resource competition	$\Delta res_i = (\beta_i / \Sigma^n_{j=1} \beta_j) * Res_{cell}$	$ms_{hoot/root}$ – shoot/root mass [mg dry weight]
Asymmetric competition	$\beta_i = ru_{max} * m_{shoot} * f_{leaf}^{-1}$	Res_{cell} – resources in cell ru_{max} – PFT specific maximal resource utilisation
Symmetric competition	$\beta_i = ru_{max} * (1/\sqrt{n_{PFT}})$	g – conversion rate resources to biomass
Shoot growth	$\Delta m = g * (\Delta res - c_{shoot} * f_{leaf}^{2/3} * ru_{max} * (m_{shoot}^2 / m_{max}^{4/3}))$	n_{PFT} – number of neighbouring PFTs
Root growth	$\Delta m = g * (\Delta res - RAR * ru_{max} * (m_{root}^2 / m_{max}^{4/3}))$	m_{max} – PFT specific maximal plant mass [mg dry weight]
Density dependent mortality	$p_{mort} = p_{base\_new} + (w_{stress} / surv_{max})$ $p_{base\_new} = p_{base} * (1 + e^{(5 * current\_abundance / max\_abundance)})$	w_{stress} consecutive weeks under stress $surv_{max}$ - PFT specific maximal survival under stress [weeks] p_{base} – base mortality (0.7%) current_abundance – current abundance of a PFT max_abundance – maximal potential abundance of a PFT (assuming fully grown individuals)

Mooij, 2005). Lateral plant growth is considered for PFTs exhibiting clonal growth. One spacer can grow per clonal PFT individual. 5% of the acquired resources are allocated to the growth of the spacer. The direction in which the spacer grows is chosen randomly from a uniform distribution. The distance of spacer growth is randomly chosen from a normal distribution based on the type-specific mean distance (SpacerL). If the determined distance the spacer has to grow is reached and the respective cell is not the centre of another individual, spacer growth stops and the new ramet can establish with a fixed probability (p_{ram}). If the reached cell is occupied by the centre of a different plant, spacer growth continues randomly within a radius of two cells.

Mortality

Plant individuals die due to consecutive weeks of resource stress (trait dependent), stochastic background mortality (density dependent), or during winter dieback. The closer the plant individuals get to their maximum survival time under resource stress (i.e. lack of resources to maintain base metabolism), the higher their mortality probability. Additionally, we added density dependent background mortality to the base background mortality of 0.7% per week corresponding to an annual mortality rate of 20 % (Schippers et al., 2001). To avoid unrealistic population densities background mortality increases exponentially if the abundance of a PFT reaches the maximum possible abundance of fully-grown individuals (i.e. a monoculture), (see 7.3.2). During winter, the aboveground biomass of each plant is decreased by 50% simulating winter dieback. If the biomass of a plant is below 10 mg, the plant is considered dead and is removed from the grid. Seeds have a probability of 50% to die during winter.

Abiotic factors

Above- and belowground resources (e.g. nutrients and light) are distributed homogeneously in space and time, i.e. we model no gradients of abiotic factors within the simulated 3 m^2 patch nor temporal changes of abiotic factors within the growing period. IBC-grass includes biotic disturbances such as grazing, trampling or cutting (see ODD-protocol for detailed information).

Temporal dimensions

One time step in IBC-grass represents one week with a total of 30 growth weeks (i.e. vegetation period) simulating one year. At the beginning of a simulation, it takes several years until a stable PFT community is reached. This is mainly explained by environmental filtering and competition between PFTs. After 150 years, the PFT community is within a stable state. As a reference, we run the model for another 25 years before we start simulating herbicide exposure effects in year 175.

4.3.3 Modelling herbicide exposure in the landscape – Xplicit

Schad and Schulz (Schad and Schulz, 2011; Schad, 2013) developed a model, Xplicit, which simulates herbicide exposure overtime and space taking into account different use rates, wind directions, application technologies and landscape structures. In our approach, we use Xplicit to simulate the drift of a broad spectrum herbicide (i.e. non selective, affecting a broad range of weed species), which has a half-life period (DT50) of 10 days, i.e. after 10 days half of the herbicide is decomposed. The typical use pattern consists of two applications per year: one application with a field dose of 739.76 g/ha and a second application with a field dose of 594.05 g/ha. Xplicit derives the variability of spray drift deposition (distance dependent) from drift models. In our approach, we use the established drift model AgDRIFT (Bird et al., 2002; Hewitt, 2002; Hewitt et al., 2002; Teske et al., 2002),

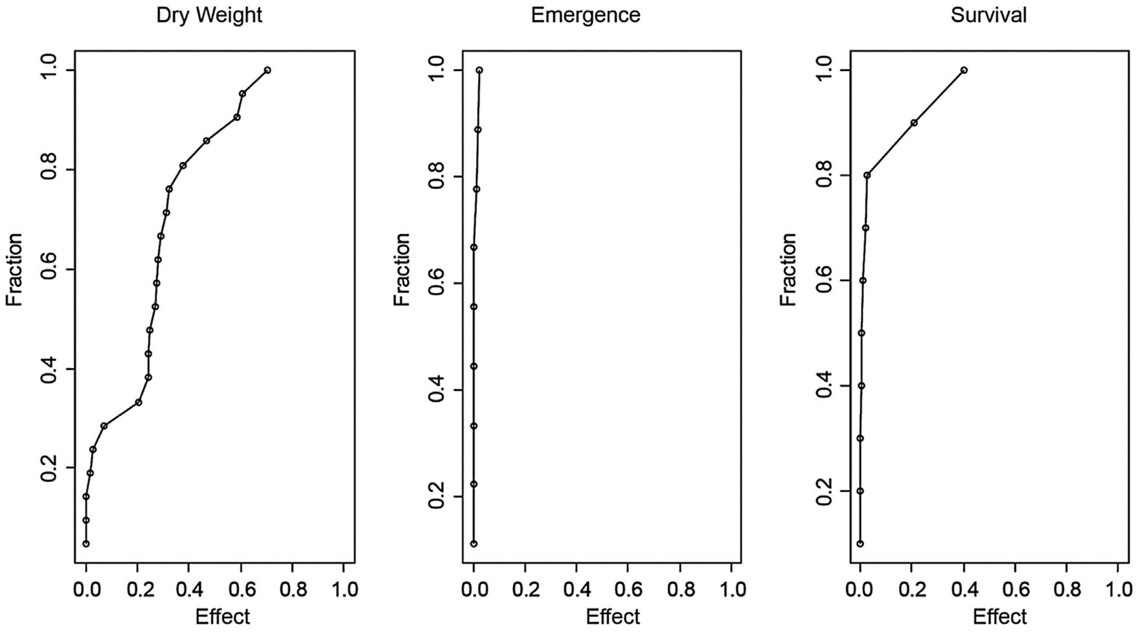

Figure 4.2: Example of species effect distributions (SEffDs) for attributes 'Shoot Dry Weight', 'Emergence' and 'Survival'. SEffDs are based on the standardized greenhouse experiments, in which at least 6 plant species (selected of a list of suitable monocotyledonous and dicotyledonous plant species (OECD, 2006a, b)) are oversprayed with different herbicide rates. Taking into account the simulated herbicide exposure on a patch in the off-field landscape, herbicide effect rates ('Effect', x-axis) can be calculated.The SEffD graphs show the cumulative effect distributions of selected species ('fraction', ordinate): e.g. for 80% of the species reduction in dry weight is ≤40%. Herbicide susceptibility is synonymous to this fraction. A PFT with a susceptibility of 0.8 will get an effect rate on dry weight of 0.4. Graphs show SEffDs for a patch in direct neighbourhood to the agricultural field.

Table 4.5: Maximum herbicide load each year within the different patches according to Xplicit calculations.

Patch distance [m]	Maximal herbicide load/year [g/ha]
1	72.149
2	32.784
3	20.266
4	14.324
5	10.916
6	8.732

which is frequently used in risk assessments for instance by US Environmental Protection Agency. AgDRIFT is a complex drift model containing several options for calculating drift by e.g. aerial, ground and orchard application. It considers e.g. droplet size distribution and boom height (Hewitt, 2002). As a worst-case scenario, west-wind conditions are assumed, i.e. wind is going directly into the neighbouring field boundary, without drift reducing technologies. No special landscape structures, e.g. slopes are considered. The simulated herbicide exposure in the landscape is variable in space but constant over the years. All plants in the field boundary community receive full spray-drift deposition (i.e., no 'in-community' variability due to spray-drift filtering e.g. higher leaf layers intercepting herbicide before it reaches lower leaf-layers). The herbicide distribution within one IBC-grass patch is homogeneously.

CALCULATING INDIVIDUAL-LEVEL EFFECTS BASED ON HERBICIDE EXPOSURE

In standard ecotoxicological dose-response tests (OECD, 2006a, 2006b) the effect of certain herbicide loads on seed mortality and seedling growth (survival, dry weight and emergence) and vegetative vigour (survival, dry weight, shoot height) are tested for a defined number of selected plant species (OECD, 2006a, 2006b). Based on this data, the effects on a given tested species under various doses are estimated by dose-response curves (OECD, 2006a, 2006b). Combining the maximum herbicide exposure within a year on a patch in the landscape (as calculated by Xplicit) and the dose-response curves, we are able to calculate species effect distributions (SEffDs): The tested species are ranked and plotted over their effects for a given herbicide dose. In doing so, we are able to calculate individual-level effects on off-field patches within the agricultural landscape context (Fig. 4.2 as example, SEffDs of all simulated patches and endpoints can be found in 7.3.3, 7.19). Our tested broad spectrum herbicide shows strongest effects on biomass, followed by effects on survival. Emergence shows lowest effect rates. We selected 6 patches within a simulated landscape differing in their distance to the field boundary (1–6 m). The specific maximum herbicide loads in the different distances are presented in Table 4.5.

HERBICIDE EXPOSURE EFFECTS IN IBC-GRASS

To include the effects of herbicide exposure on plant individuals in IBC-grass, we extend the model with toxicological sub-processes. In this way, growth, mortality and establishment of seedlings and adult plants are influenced by the herbicidal effect rates in accordance with the SEffDs based on OECD guideline endpoints (OECD, 2006a, 2006b) taking into account PFT specific herbicide susceptibilities(see *Species specific susceptibilities*).

- After normal plant growth is calculated, biomass is reduced by the specific effect rate.
- After plants suffered from the stress-induced and/or demographic-related mortality, additional herbicide-induced mortality is included with the specific probabilistic effect rate.
- Seedling mortality is increased by the specific probabilistic effect rate.
- Seedling biomass is reduced by the specific effect rate after the seedling is established.
- After seeds suffered from the demographic-induced mortality, additional herbicide-induced mortality occurs with the specific probabilistic effect rate.

In the standard non-target terrestrial plant studies for the herbicide used in this modelling exercise, effects on dry weight and shoot length are measured (acc. to OECD and USEPA Guidelines(USEPA, 2012a, 2012b; OECD, 2006a, 2006b)). However, in IBC-grass we do not consider shoot length directly, but indirectly by correlating biomass and growth form in the ZOI approach. In order not to underestimate the effect, we select the most sensitive endpoint which is dry weight in our case study. Furthermore, due to the way growth is calculated in the model, it was not possible to relate the effect on dry weight to a growth rate (which would directly reflect the outputs of the guideline studies) but the effect has to be concentrated into one week and affected biomass directly. Therefore, effects on biomass can be assumed as very conservative and potentially overestimated.

SPECIES SPECIFIC SUSCEPTIBILITIES

Herbicide susceptibility varies among different plant species, e.g. due to secondary metabolites, specific plant features like hairiness of leafs (Prather et al., 2000) or the mode of action of the compound. A broad range of plant species would need to be tested for each compound. This is partially fulfilled by conducting standard non-target terrestrial plant guideline studies but to further account for the wide variety of plants those tests would become very time consuming, expensive and labour intensive. In addition, the handling of some plants is not practical or the tests are not feasible (e.g. unsuitable growth form such as ranking plants, high variation, low germination probability, etc). Therefore, only selected plant species are considered for standardized greenhouse experiments, which are deemed appropriate to cover the range of possible sensitivities when an assessment factor is considered (Christl, 2015).

This also holds true for our case study compound, where dose-response tests were conducted for standard test species only. Therefore, we are not able to assign any verified herbicide susceptibilities to our PFTs. As a temporary conservative work-around we assign herbicide susceptibility randomly among the PFTs in our regional pool. We use a uniform distribution of herbicide susceptibility varying between 0 and 1. For each Monte Carlo run, herbicide susceptibility is assigned anew to cover a maximum range of possible susceptibility distributions. The resulting high variability allows for the identification of general response pattern that do not depend on specific susceptibility distributions.

4.3.4 Simulation scenarios and analyses

We simulate worst-case scenarios, in which herbicide exposure occurs over a period of 30 years (1 application per year) under conservative conditions, i.e., during the application of the herbicide on the arable field wind is coming directly towards the examined field boundary, and no drift-reducing technologies are applied. To account for potential recovery effects, these 30 years are followed by a period of 35 years without any herbicide exposure. A scenario without any herbicide exposure serves as control. Each scenario is repeated 50 times (i.e. 50 Monte Carlo runs (MCs)) to account for the high stochasticity of the model.

We analyse the effects on (i) population size on population level within community context and the effects on (ii) aboveground biomass, (iii) PFT richness and (iv) diversity on community level. The following analyses are conducted: For each patch and evaluation variable (see above), the mean (per week and year) of the control scenario is calculated and used as a reference for standardization. The values of all evaluation variables of all 50 treatment and 50 control MCs are standardized by the reference (per week and year). For each year, the 2.5th and 97.5th percentile of the standardized control MCs are selected as a measure of standard variation of population size, aboveground biomass, PFT richness and diversity within the community. On community level, standardized values of treatment MCs are plotted per year in boxplots. If the median is out of the range of standard variation, we consider it a significant effect (which should not to be confused with the concept of statistical significance). On population level, we plot the mean of all standardized treatment MCs per week and year to show the temporal dynamics within and between years.

4.4 Results

4.4.1 Effects on community level and differences between plant communities

Looking at the behaviour of community-level evaluation variables in the course of time for one scenario of the simulated *Calthion* community, aboveground biomass is significantly decreased during the week of herbicide drift exposure and recovers over the year i.e. one growing period (Fig. 4.3). However, it is not completely recovering each year resulting in a slight decrease of aboveground biomass between the years. Only minor effects can be observed for PFT richness: it slightly increases after herbicide exposure but decreases over the years. However, the variation within the control simulations indicates that these effects are within the normal variation of PFT richness in the presented community. In contrast, strong effects can be detected on diversity (represented via the inverse Simpson index, taking into account PFT richness and abundance). There is a strong decline within the presented time frame. However, the index shows a relatively high fluctuation already in years without herbicide exposure.

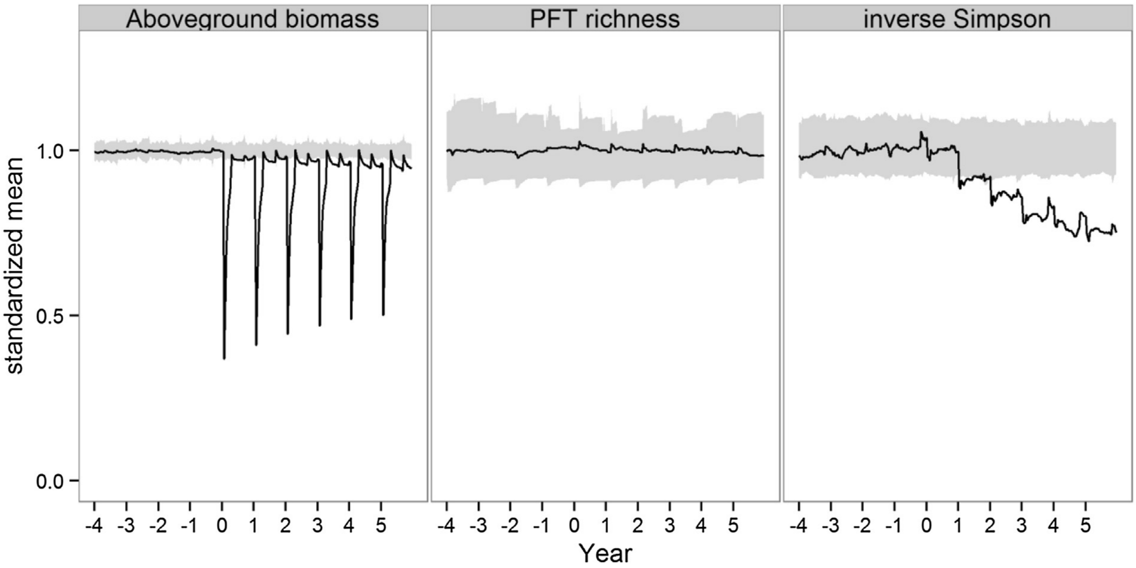

Figure 4.3: Timeline of herbicide drift exposure effects on community-level for *Calthion* community on a patch in 1 m distance. The continuous line represents the mean ofstandardized values (by the weekly mean of 50 control simulations) of each week per year for 50 treatment simulations. A standardized value of 1 means, that there is nodifference between control and treatment. Grey background ribbons showing the 2.5th and 97.5th percentile of standardized control simulations. Graphics show 4 years before treatment and the first 6 years of simulated herbicide exposure (starting at year 0). I.e. a decrease by 0.5 means an average reduction e.g. in aboveground biomass of 50%.

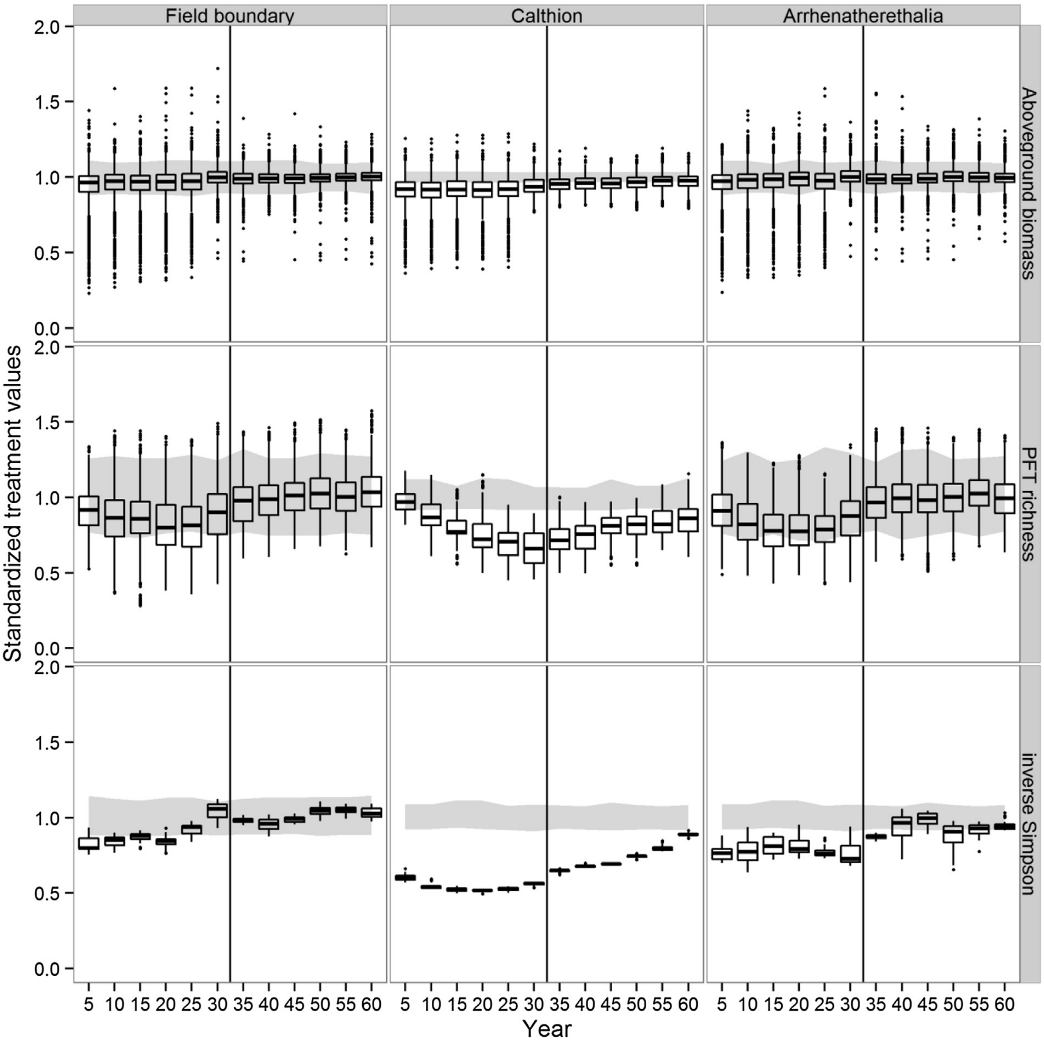

Figure 4.4: Differences in communities regarding herbicide drift exposure effects on community-level for total aboveground biomass, PFT richness and inverse Simpson index on a patch in 1 m distance. Boxplots represent standardized values (by the weekly mean of 50 control simulations) of each week per plotted year for each of the 50 treatmentsimulations (i.e. one boxplot consists out of 1500 standardized values). For reasons of readability only every 5th year is plotted. A standardized value of 1 means, that there is no difference between control and treatment. All outliers are presented. Grey background ribbons showing the 2.5th and 97.5th percentile of standardized controlsimulations. Herbicide treatment was simulated for 30 years, as indicated by the vertical line, followed by 35 years of potential recovery (without herbicide treatment).

Communities differ in their natural variability; the field boundary community and *Arrhenatheretalia* community display more variability than the *Calthion* community indicated by more outliers in periods without simulated herbicide treatment (year > 30)(Fig. 4.4). Strongest effects can be observed in the *Calthion* community for PFT richness and inverse Simpson index. Diversity is significantly decreased (i.e. boxplots outside of ribbon). Field boundary community and *Arrhenatheretalia* community show similar effects of simulated herbicide drift exposure. Aboveground biomass is strongly decreased in few weeks per year (represented by a higher amount of outliers (one outlier = one week within a treatment simulation)), but is not significantly decreased in the long-term. Aboveground

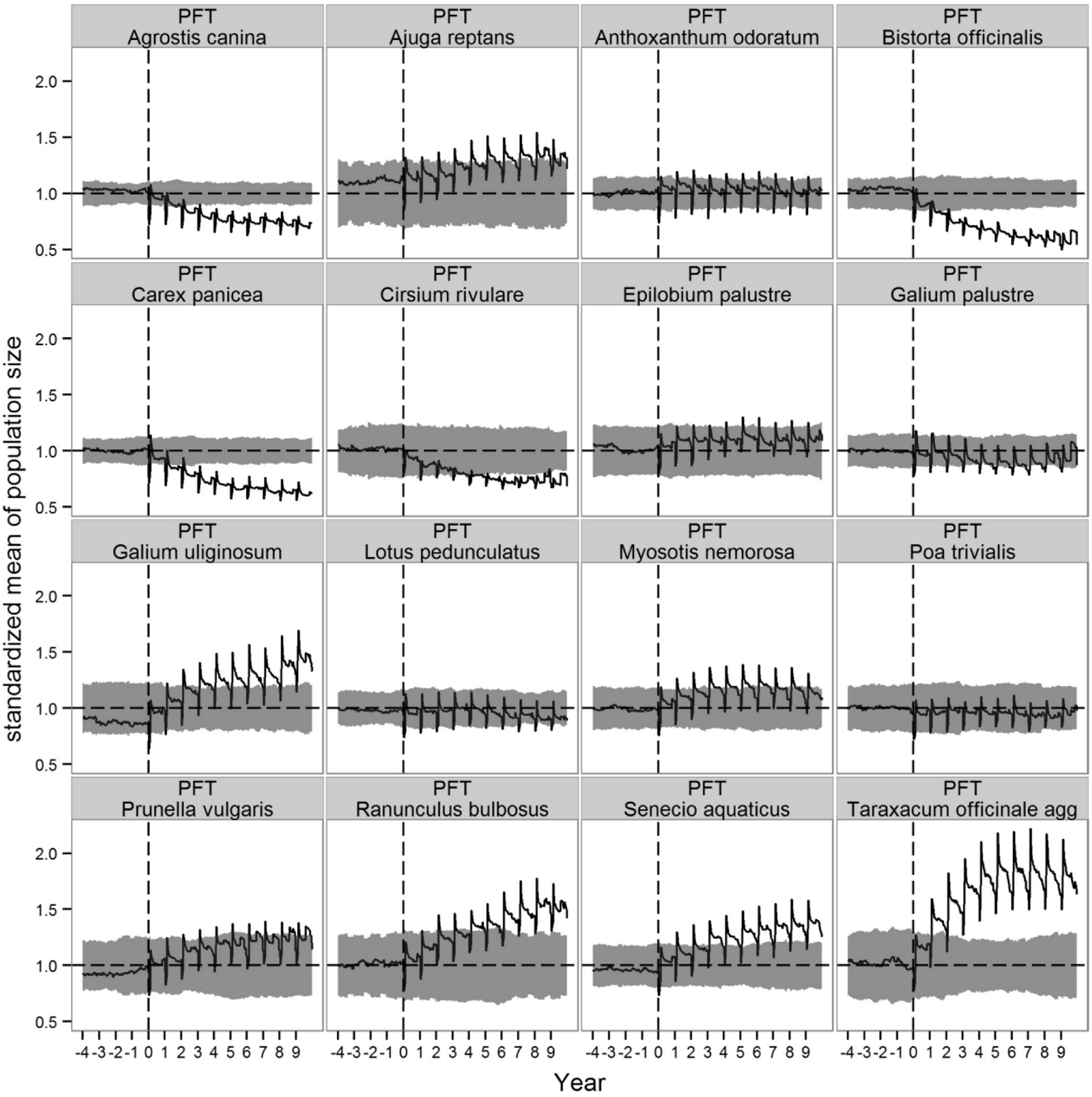

Figure 4.5: Herbicide drift effects on PFT population sizes within community context for *Calthion* community on a patch in 1 m distance (other communities shown in 7.3.3 ,Fig. 7.20 and 7.21). In this case the PFTs are represented by a certain plant species which belongs to the PFT group. Solid lines represent the standardized mean (standardized by the weekly mean of 50 control simulations) of each week per year out of 50 treatment simulations. A standardized mean of 1 means, that there is no difference between control and treatment. Grey background ribbons showing the standard deviation of standardized control simulations. For a better visualization of thetemporal dynamics, only the last 5 years before herbicide drift exposure and 10 years during herbicide exposure and only PFTs with a mean frequency (in control simulations) of >0.9 are presented. Population dynamics over the whole simulated period (30 years herbicide exposure followed by 35 years 'recovery' without exposure can be found in 7.3.3 Fig. 7.23).

biomass recovers completely if herbicide treatment is suspended. In addition, PFT richness is slightly decreased by herbicide drift exposure. Effects are not significant for all simulations and the whole year, i.e. PFT richness is able to almost recover within a year. But the trend of the 30 years of repeated herbicide exposure suggests that there probably will be significant long-term effects on the PFT richness (median values constantly decreasing). Nevertheless, PFT richness is able to recover within a few years of suspended herbicide exposure. However, significant effects are detected for diversity, which not only considers PFT richness, but also abundance of PFTs. For the field boundary community, inverse Simpson-index is first strongly declining, but able to steadily recover. Considering the decline in PFT richness, this indicates a shift in community composition. Within the *Arrhenatheretalia* community, significant effects can be detected on biodiversity, but there are high fluctuations even when herbicide treatment is suspended. Therefore, the field boundary community has a slightly higher recovery potential than the *Arrhenatheretalia* community.

4.4.2 Effects on population level

Since *Calthion* shows highest sensitivities, population level results are shown only for *Calthion*; however, results for other communities can be found in 7.3.3, Figs. 7.20 and 7.21.

As expected, all PFTs show an immediate negative response to herbicide exposure (e.g. peaks at the beginning of each year, Fig. 4.5). Over the long term, three PFTs show a decline in population sizes over the year (PFT *Agrostis canina, Bistorta officinalis, Cirsium rivulare* and *Carex panicea*). However, in four cases (PFT *Galium uliginosum, Ranunculus*

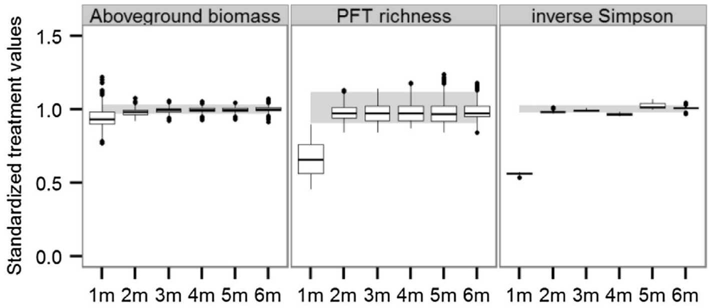

Figure 4.6: Drift exposure effects on community level of the *Calthion* community at varying distances to the arable field after 30 years of simulated herbicide application. Boxplots represent standardized values (by the weekly mean of 50 control simulations) of each week per year for each of the 50 treatment simulations (i.e. one boxplot consists out of15,000 standardized values). The graphic shows the last year of 30 years repeated herbicide application. A standardized value of 1 means, that there is no difference betweencontrol and treatment. All outliers are presented. Grey background ribbons showing the 2.5th and 97.5th percentile of standardized control simulations. The x-axis 'distance'indicates the potential herbicide exposure extent according to Xplicit calculations. However, community dynamics in IBC-grass are still simulated on a 3 m^2 patch.

bulbosus, Senecio aquaticus and *Taraxacum officinale* agg.), the mean standardized population size increases over time, i.e. the PFT recovers from the immediate herbicide effect within the year and even more individuals are able to establish in the community. In this respect, also infrequent PFTs show several occurrences where standardized population sizes strongly increase during some weeks (see 7.3.3, Fig. 7.22).

4.4.3 Distance to field

The effect of herbicide drift exposure strongly decreases within the first meter distance to the arable field (1–2 m). In the adjoining2–6 m distance, there is only a slight reduction of effects (Fig. 4.6). Here, herbicide exposure is already diminished.

4.5 Discussion

Our simulation scenarios demonstrate that herbicide depositions can have complex effects on non-target plant communities. These effects differ for the different communities. We test three plant communities in nutrient rich to medium environments with high to medium disturbance levels by mowing and trampling activities. Among the simulated communities, the *Calthion* community shows the highest sensitivity towards herbicide deposition. A *Calthion* grassland is characterized by medium to low nutrient levels and is typically managed as a meadow with only one cut per year (Dierschke et al., 2004). Therefore, plant species occurring in such grasslands are rather poorly adapted to disturbances. The main driver in such systems is the adaptation of plants to comparably low resource levels (Aerts, 1999). Introducing herbicide deposition to these communities causes loss of biomass and increases mortality, similar to effects of increased grazing and mowing. In response, plant species specialized to low disturbed but resource-stressed environments are replaced by species that are able to recover faster from disturbance events. Contrastingly, the field boundary plant community and *Arrhenatheretalia* grassland are characterized by high nutrient levels (due to fertilizer deposition/input) and higher disturbance events (e.g. farmer's activities on a field boundary and three cutting events on an *Arrhenatheretalia* meadow (Dierschke,2004; Fischer, 1985)). The main aspect, which drives the dynamics of these plant communities are disturbance events, since resources are not the limiting factor (Aerts, 1999). Thus, the addition of herbicide deposition as another disturbance agent does not change species composition over the long-term. Frequent plant species in these communities are already adapted to high disturbances and therefore, can cope better with herbicide deposition events than species in a less disturbed community such as *Calthion*.

The indirect effects of herbicide deposition, which result in the change of species composition, can best be observed on population level. Over the long-term, single PFTs show either a negative, positive, or neutral effect on population size. During the herbicide exposure in the period of germination, all PFTs show a negative effect. However, as the year progresses, population sizes show different trends. For example, PFTs *Agrostis canina, Bistorta officinalis, Carex panicea* and *Cirsium rivulare* are not able to recover completely within a year. Consequently, their population sizes are decreasing over the years. All of these PFTs include plant species with medium to large maximal plant sizes, semi-rosette growth forms and adaptations to resource stress. These species can survive low resource uptakes for a longer time period. However, the combination of high maximal plant sizes and a semi-rosette growth form results in lower growth rates as a trade-off. Plant individuals of these PFTs need longer to rebuild biomass after a disturbance event and, in addition, produce fewer seeds (with higher seed masses) (Grime, 2001). Although seeds with higher seed masses have a competitive advantage in establishment (Schippers et al., 2001), they also have lower chances in dispersing into empty establishment sites as they have smaller dispersal kernels. Therefore, replacing deceased individuals with new seedlings is a low probability. In contrast, population sizes of the PFTs *Galium uliginosum, Ranunculus bulbosus, Senecio aquaticus* and *Taraxacum officinale* increase over the years. These PFTs are characterized by small plant sizes and show no adaptation to resource stress. Correlated to their small plant sizes, these species produce many small seeds, which have a wide dispersal range. Therefore, there is a higher chance for seedlings to establish, hence, compensating the increased mortality of single individuals.

Herbicide deposition effects on plant communities are not only depending on the mode of action of the compound, management, species pool and certain traits, but also on the distance to the arable field. The fraction of herbicide in a certain distance to the arable field depends on the herbicide-specific application method, the wind direction and intensity and the distance to the last nozzle (Wang and Rautmann, 2008). Therefore, on patches directly located at the field boundary, a higher herbicide deposition can be observed and, correspondingly, also stronger negative effects on the community. A distance of 3–6 m is often considered as a buffer zone in herbicide risk assessments (de Snoo, 1999). This is in accordance with the findings of our simulation experiment. At a distance of 3 m, IBC-grass detects only negligible effects on community level (Fig. 4.6).

Spray drift interception by taller plants or other exposure routes, e.g. vapour drift or run-off, could be other important mechanisms of individual plant exposure that could have impacts on relative PFT population responses and thus also on community composition and response patterns. Implementing this additional variability into the IBC-grass would add an additional level of complexity. Since the current version of IBC-grass mainly aims at a first basic demonstration of its potential to scale up from individual effects to populations and communities these and other additional aspects will be investigated in a future version of the model.

Due to the lack of information on PFT specific herbicide susceptibilities, we assign this parameter randomly in each Monte Carlo run (MC), i.e. the complete range of PFT susceptibility is sampled. Therefore, variability between MCs is strongly increased and one could expect that effects seen in single runs level each other (e.g. MCs in which a certain PFT suffers less compensates for MCs in which this specific PFT suffers more due to assignment of higher herbicide susceptibility). However, in spite of these artificially assigned susceptibilities, several PFTs show a clear positive or negative feedback on herbicide deposition. This indicates that the IBC-grass model is rather robust to detect possible herbicide deposition effects although species specific herbicide susceptibilities remain uncertain. In other words the impact on species in a community is more related to their life strategy and the resulting traits than to their specific sensitivity to the pesticide. However, the understanding of the plant species' susceptibility to herbicides should be deepened and enlarged. Future studies should focus on plant traits that may lead to lower or higher susceptibilities (see Rubach et al., 2010 for a conceptual approach). Boutin et al. (2012) studied the relationship between herbicide efficiency and certain plant traits, which potentially influence the efficiency. They were not able to find any correlation between the measured traits and the efficiency. However, they agreed that further research is needed since they only tested a few of several traits, which might influence herbicide susceptibility. In IBC-grass, future modelling studies should also focus on grouping PFT herbicide susceptibility according to specific trait characteristics, e.g. distinguishing between monocotyledonous and dicotyledonous species.

In addition, we face a general problem in translating the effects on the biomass into IBC-grass. Within standard ecotoxicological studies, effects on dry weight are measured 7, 14 and 21 days after exposure at the 2–4 leaves growth stage. Effects on older plant individuals are not investigated, since they are assumed to be covered by the more sensitive juvenile stages. However, also plant individuals in advanced growth stages will experience effects on biomass. Due to a lack of data on older individuals within the ecotoxicological experiments, we apply the full effect extents on all plant individuals, disregarding the individual, plant age specific growth rate. Therefore, older plant individuals might be assigned a greater effect than in the real-world. Eventually, further research is needed to investigate the decrease in effect extent for older plant individuals for more realistic effect patterns.

Several studies conducted experiments to test the effects of various herbicides on plants with different modes of actions (e.g. Damgaard et al., 2011; Pfleeger et al., 2012; Riemens et al., 2008).These studies focused either on the differences between crops and weeds (e.g. Carpenter and Boutin, 2010), sublethal and reproductive effects (e.g. Wagner and Nelson, 2014) or the sufficiency of standardized regulatory risk assessment tests (e.g. Kleijn and Snoeijing, 1997). However, few studies tested effects on community level in realistic field/(semi-)field experiments. Kleijn and Snoeijing (1997) did a field experiment over two years. Similar to our simulation experiments, they detected different herbicide exposure effects for different plant communities especially due to species composition and nutrient levels. However, the authors highlighted that management regimes (mowing, grazing) may be of more importance than herbicide exposure. Since we regard different plant communities with different management regimes, we are able to confirm that management regimes might indeed be a decisive factor for the composition of plant communities in cultivated landscapes, dominating over the effect of herbicide exposure on a plant community. Marrs and Frost (1997) did a microcosm approach with standardized species assemblages which lasted for3 years. They found similar patterns compared to our results. With increasing distance, herbicide drift effects were diminished and they found positive feedbacks of some species, which was related to reduced competitive pressure. More recent studies also found similar results (e.g. Damgaard et al., 2014; Schmitz et al., 2014). However, all of these studies were carried out for not longer than three years. Real long-term effects and trends could not be observed. Kleijn and Snoeijing (1997) even mentioned the high variability between years. Our results show that the intensity of effects is increasing over time and potential risk of extinction for some PFTs can be only seen after several years. Model approaches have the advantage to incorporate long-term investigations and higher amount of repetitions, thereby capturing the high natural variability of real-world plant communities and long-term effects of herbicide drift exposure.

4.6 Conclusion

In this study, we give a first impression of the potential and possibilities of using a spatially-explicit, plant-functional and individual-based modelling approach to extrapolate individual-level effects of non-target herbicide exposure measured in greenhouses to plant community level within the landscape. Using simulated effects of a broad spectrum herbicide, which acts on all plant species, as a first general application we show how effects on plant individuals can lead to both direct and indirect community responses by modifying population dynamics and relative interaction networks. The chosen trait- and individual-based modelling approach will also allow including and exploring more refined scenarios (e.g. selective herbicides, which act only on monocotyledonous or dicotyledonous species) and more detailed processes (e.g. increased herbicide interception by taller plants) in future versions of IBC-grass. In part, this will have to be accompanied by additional experiments such as susceptibility measurements for a broader range of herbaceous species.

Overall, mechanistic modelling approaches such as IBC-grass can help to improve our understanding of the complex interactions within grassland communities. We show that they also present a promising approach in transferring and extrapolating standardized pot experiments (as regulated in e.g. the OECD guidelines 208 and 227 (OECD, 2006a, 2006b)) to population and community level and thereby bridging the gap between ecotoxicological testing (e.g. in the greenhouse) and protection goals referring to real world conditions.

5 General discussion

Non-target terrestrial plant communities can have various appearances (Marshall and Moonen, 2002). What all communities have in common is that they are located in direct neighbourhood to arable fields and thus potentially threatened by unintended exposure of pesticides, e.g. due to drift. In this thesis I focused on herbaceous plant communities potentially occurring at field margins in Germany and the impact of herbicide drift exposure on the population and community dynamics. I chose a modelling approach to address knowledge gaps and to obtain clarity in the uncertainties of current risk assessments for these non-target terrestrial plant communities.

In the first study[1] of my thesis I was able to show that the plant community model IBC-grass was able to predict similar effect patterns on aboveground biomass as observed in the experimental study by Reuter and Siemoneit-Gast (2007). Firstly, the model was able to realistically address inter- as well as intraspecific competition within monocultures and artificial communities. Secondly and most important for the objectives of my thesis, the study demonstrated the suitability of the model to evaluate the consequences of herbicides on non-target plant communities. In the second study[2], I went a step further and approached the uncertainty of the current endpoints used in the risk assessment, namely shoot dry weight, mortality and seedling emergence, for the protection of non-target terrestrial plant communities. Several researchers requested to integrate reproductive endpoints as their studies showed a higher sensitivity for these endpoints compared to the vegetative vigour endpoints currently used (Boutin et al., 2004; Carpenter et al., 2013; Riemens et al., 2009, 2008). Indeed, seed production is an important driver especially for annual plant populations (Turnbull et al., 2000). However, the questions is to which degree a reduction of seed production can be tolerated and compensated by other mechanisms such as seed dispersal or a seed bank. My study showed that only very high impacts on seed production led to significant impacts on population and community level, even though seed bank is not considered in the model. Thus, the impact might be even higher until significant effects can be observed. In contrast, already a minor impact on plant mortality or on seed sterility led to significant effects on population and community level. These endpoints are already included in the current guidance. In conclusion, only if strong impacts on seed production or the seed sterility of the F1 generation are expected (e.g. due to the mode of action), reproductive endpoints should be considered in risk assessments. Finally, the third study[3] highlighted the importance of not only considering

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[1] published as: Reeg J, Heine S, Mihan C, McGee S, Preuss TG, Jeltsch F. 2018. Simulation of herbicide impacts on a plant community: comparing model predictions of the plant community model IBC-grass to empirical data. Environ Sci Eur 30:44

[2] published as: Reeg J, Heine S, Mihan C, Preuss TG, McGee S, Jeltsch F. 2018. Potential impact of effects on reproductive attributes induced by herbicides on a plant community. Environ Toxicol Chem. 37(6):1707-1722

[3] published as: Reeg J, Schad T Preuss TG, Solga A, Körner K, Mihan C, Jeltsch F. 2017. Modelling direct and indirect effects of herbicides on non-arget grassland communities. Ecological Modelling. 348: 44-55

individual-level effects but also pay attention to plant populations in community context, i.e. including inter- and intraspecific competition. In the study, I showed that herbicide impacts can result in indirect effects on plant populations within community context. Interspecific competition and trait characteristics influenced the impact of the theoretical herbicide for PFT populations in the community context: PFTs adapted to stressful environments, e.g. by high seed production or high growth rates, were able to recover fast from the negative herbicide impact and showed a positive impact over the long-term, whereas PFTs with low growth rates and low seed production were not able to recover within a year and thus showed a negative impact. The results of this study showed a shift in community structure under herbicide drift exposure. Plant communities which were already adapted to disturbances showed weaker shifts in PFT composition than community not adapted to disturbances. This result is in agreement with the EFSA scientific opinion that specific protection goals for non-target terrestrial plants must be considered in order to meet the EU Regulation 1107/2009 for pesticide authorization that there shall not be unacceptable impact on the environment (EFSA PPR Panel, 2014a; EC, 2009a).

In the following I put my studies in the broader context of herbicide risk assessment of non-target plants and the risk regulation in the European Union. First, I discuss the ability of this modelling approach to be transferred to different herbaceous field boundaries and environmental conditions and thus to allow for general conclusions. Next, I focus on plant-plant interactions in the plant community and the resulting indirect impacts of herbicide exposure that are neglected in the current risk assessment of non-target terrestrial plants. I continue to compare the IBC-grass model with other existing plant population or community models used in ecology and the lack of models used in ecotoxicology. I elaborate on the use of ecological models in herbicide risk assessments focusing especially on the hesitation of using models as alternative higher tier study. I propose an option how the empirical data of the current OECD 208 and 227 guidelines (OECD, 2006a, 2006b) can be transferred to the IBC-grass model to extrapolate these individual-level effects to a community level. Finally, I give a short summary of alternative mitigation measures, followed by an overall conclusion and future perspectives.

5.1 Extrapolation to other grasslands

Terrestrial plant communities in direct neighbourhood to arable fields are highly variable in their composition between countries and even within one country owing to different environmental conditions, agricultural managements and regional species pools (Aavik et al., 2008; Kleijn and Verbeek, 2000). Thus, it is difficult to find a reference community which can reflect the variety of different species composition of herbaceous field boundaries in the zonal regions of the European Union. Using a trait-based modelling approach as I did in my thesis is a suitable method to reflect several different regional species pools. One PFT can combine the behavior of not only one but several plant species with similar trait characteristics. Thus, trait-based approaches can be the solution to extrapolate risk assessments across geographical regions (Baird et al., 2008) and to summarize several species composition within one PFT composition.

The regional species pool includes plant species adapted to the geographical region and its climatic and abiotic as well as biotic conditions. Thus, different ecological processes drive the plant community dynamics. To reflect a high variety of environmental conditions and thus different regional plant communities, an ecological model needs to include various different processes that potentially act on the plant community dynamics. Biotic disturbances are well reflected in the IBC-grass model. Grazing by small and large herbivores, trampling effects due to agricultural activities or large mammals and mowing events, e.g. to manage field margins, can be adjusted. These processes are known to have a high impact on plant community composition and dynamic in general (Olff and Ritchie, 1998; Tälle et al., 2016). Currently, abiotic conditions are summarized into overall above- as well as belowground resource levels, distributed homogeneously in space and time. This is a valid assumption for climatic conditions in large areas of the central zonal areas in Europe, like Germany. Weiß et al. (2014) showed that the model realistically reflected the patterns of aboveground biomass for grasslands with varying grazing intensity in Germany. However, regions at the edge of the temperate zone are characterized by harsher environmental conditions (e.g. dry summer in Spain and harsh and longer winter in Sweden). For these regions, a refinement of distribution of resources in time might be necessary to realistically predict plant community dynamics. Furthermore, especially on a local scale, a refinement of resources and the correlated adaptions of plant species can increase the applicability of the model for a wider range of field boundaries. In the Netherlands, for example, agricultural fields are often surrounded by ditches. Thus, the soil moisture gradient is important for community dynamics and probably needs to be integrated before the model can be applied to these specific environmental conditions. Schibalski et al. (2018) adapted the IBC-grass model for coastal grasslands by integrating the adaption to salinity and water stress, indicating the potential of IBC-grass to be adapted to several different environmental conditions.

However, ecological models are designed to simplify the real world by detecting the main drivers for, e.g., plant community dynamics. Adding complexity to a model needs to considerably increase the performance of model predictions. Thus, it should be first tested, whether the original model version is able to reflect field boundaries in specific regional or local areas before extending the model with further processes.

5.2 The lack of accounting for plant-plant interactions in current risk assessment of non-target terrestrial plants

Plant-plant interactions are known to be important for community dynamics (Gotelli and McCabe, 2002) and changes in the competitive ability of plant individuals shifted the impact on community level as shown in chapter 4 of my thesis. Damgaard et al. (2011) investigated the competitive growth of *Festuca ovina* and *Agrostis capillaris* under the impact of glyphosate and nitrogen. The treatments had significant impacts on the competitive growth and increased the sensitivity of *A. capillaris* in the community context. This is in agreement with the studies by Riemens et al. (2008, 2009), which showed that plant individuals grown in mixtures had different sensitivities towards the herbicide Aramo (active ingredient: Tepraloxydim) compared to individually grown plants. These empirical studies showed that indirect effects caused by plant-plant interactions must be considered to realistically predict herbicide impacts on plant community level. However, plant-plant interactions are neglected in the current risk assessment of non-target terrestrial plants.

The EFSA acknowledged that also indirect competition between individuals can lead to indirect effects shifting the impact on the diversity at community level. In conclusion, EFSA proposed specific protection goals (SPGs) considering, among others, also the indirect effect of herbicides within a plant community (EFSA PPR Panel, 2014a). Using the existing OECD test guidelines 208 and 227 (OECD 2006a, 2006b), the SPG should be realized using an operational protection goal described as "95% of the plant species will not be exposed above their ER10 under consideration of realistic worst case off-field scenarios" (EFSA PPR Panel, 2014a). Uncertainties, including the extrapolation from single species tests to the multiple species situation in the real world, should be addressed using either higher tier testing (e.g. additional studies testing for these uncertainties) or using adequate assessment factors. Finding adequate assessment factors require a suitable reference tier including sufficient data in terms of number of test species, communities and compounds. Thus, higher tier options can be a good alternative to meet the SPGs. The EFSA summarized several empirical study designs which could be suitable higher tier studies to account for species interactions. However, as these studies are labour intensive and request a high amount of spatial resources, they can only include a small range (<10) of test species and thus may not cover the whole range of potential species-species interactions. In addition, results of more complex studies (e.g. Schmitz et al., 2013) are often difficult to interpret as impacts of various factors driving the results cannot be disentangled. Ecological models can help to understand the influence of plant-plant interactions for the impact of herbicide drift exposure in plant communities. As shown in chapter 2 of my thesis, the plant community model IBC-grass realistically simulated plant growth in monocultures as well as in the artificial communities without herbicide impact. In addition, herbicide impacts on the aboveground biomass in the artificial communities were realistically predicted by the model. This infers that plant-plant interactions are well reflected and indirect impacts of herbicide exposure can be simulated using this modelling approach. In addition, ecological models can have a full factorial test design as they are not limited in space and time compared to empirical studies. From these modelling studies, research questions can arise that can be underlined by a suitable empirical study. To conclude, ecological models can help to design empirical studies and to select important factors that need to be included in an empirical study. Henry et al. (2017) called this approach funnel analysis, i.e. using ecological models to identify sensitive environmental stressors and conditions which can then be studied in empirical studies.

5.3 Plant population and community models in the ecotoxicological context

Recently, plant population models are given special consideration as useful tools for assessing the risk of endangered species to be affected by pesticide applications. Schmolke et al. (2017a) introduced a framework for developing population models in the ecotoxicological context using a matrix modelling approach. Matrix models categorize populations into different age or stage classes considering transition probabilities from one class to the other (Caswell, 2001). Schmolke et al. (2018, 2017b) applied this approach for two endangered herbaceous plant species, *Asclepias meadii* and *Boltonia decurrens* indicating the suitability of this approach to be used for risk assessments of endangered species. Actually, the EFSA supports the use of matrix modelling for extrapolating from individual-level to population-level (EFSA PPR Panel, 2014a) and gives a detailed example for the application of a matrix modelling approach.

Still, interspecific competition is neglected in these models, although empirical studies showed the importance of plant-plant interactions for community dynamics as discussed previously. Thus, plant population models can be used for the risk assessments of endangered species, but they cannot predict the risk at community level as they lack the interspecific competition. Despite the increasing demand for assessing pesticide impacts on community-level, there is still a lack of plant community models used in the field of ecotoxicology. However, some examples for plant community models which study ecological research questions can be found in the literature. For example, VEGPOP2 is spatial plant community model, incorporating resource competition and population dynamics (Schippers and Joenje, 2002; Schippers and Kropff, 2001). During the simulated period with one time step being one day, it tracks the number of plants per species and for each species the distribution of biomass in different parts of the plant (flower, leaf, stem and root). The model was parameterized for four plant species, representing a small community. Another example is the individual-based and spatially explicit plant community by Warren and Topping (Warren and Topping, 1999, 2004) who studied drivers of co-existence of 6 plant functional types. The particular trait characteristics and the biotic and abiotic environmental conditions determined the competitive performance of the plant individuals. The model simulates long-term dynamics as one time step represents one month. The IBC-grass model, on which I based my thesis, combines several advantages of both model approaches: Its individual-based approach facilitates the integration of individual-level effects that are measured by default during the risk assessment of non-target plants. The trait-based approach allows to make general conclusions and to transfer prediction to various communities with different regional species pools. Furthermore, the temporal resolution of one time step representing one week is a good compromise to simulate short-term but also long-term impacts on populations within the community context. In addition, the spatial resolution covers local impacts, but can also be up-scaled to a broader landscape level. For example the model can simulate different local patches within a landscape considering the distance to arable fields or other environmental gradients occurring in the landscape.

5.4 Using IBC-grass in future risk assessments

The current risk assessment scheme for non-target terrestrial plants is following a tiered approach consisting of three steps (Tier I – Tier III; EC, 2002). During an initial screening experiment (Tier I), 6-10 plant species, grown individually in pots, are sprayed with the highest application rate. If one or more plant species exhibit more than 50% effect in one of the measured endpoints, Tier II studies need to be conducted which includes testing different application rates to calculate dose response curves. If the Tier II studies still indicate unacceptable risks for terrestrial plants, Tier III studies have to be conducted, e.g. semi-field study including realistic exposure rates. Thus, realism is increasing with increasing tiers. Standard guidelines exists for Tier I and Tier II tests (OECD 2006a, 2006b).

However, guidelines for Tier III studies are still missing. A new guidance document for non-target terrestrial plants is currently under development. Based on the EFSA scientific opinion the specific protection goals will probably be on population and community level to meet the EU Directive 1107/2009 (EC, 2009a; EFSA PPR Panel, 2010). Thus, there is an urgent need for suitable Tier III options which increase the level of protection for non-target terrestrial plants. In my thesis, I propose a novel approach for a higher tier option which extrapolates individual-level effects measured in the standardized greenhouse experiments to impacts on population and community level.

The approach is based on the dose responses of Tier II studies. These individual-level effect data are transferred into the plant community model IBC-grass to predict short- as well as long-term impacts on plant populations within the community context (see chapter 2). Herbicide exposure models can be used to calculate potential drift rates at a local patch simulated by IBC-grass. Thus, realistic exposure, worst case scenarios and the influence of mitigation measures such as buffer zones can be included. However, the remaining uncertainty is the assignment of dose response curves based on the 6 – 10 test species to the plant species (or PFTs) actually inhabiting field boundaries. Christl (2015) showed that the test species cover the range of potential sensitivities of non-target terrestrial plants, but the distribution of sensitivities between the field margins might influence the impact on community level. Thus, it is important to determine whether a plant species occurring within these communities has a higher or lower sensitivity.

To overcome this gap, I propose to calculate a mean dose-response based on the dose-response functions of each test species, including the corresponding standard deviation. Assuming a uniform distribution of dose responses within this range, dose responses can be randomly drawn from that distribution and assigned to the PFTs. In the second chapter of my thesis, I calculated species specific dose responses to predict the impact on biomass at the community level (Reeg et al., 2018b). I used this data to calculate a mean dose response and random dose responses based on the mean and the standard deviation (Figure 5.1). Assigning the dose responses randomly to the PFTs instead of the PFT specific dose responses as I did in chapter 2, led to similar model predictions (Figure 5.2). This indicates that this approach is a suitable work around if the sensitivity of a plant species is unknown. However, correlating the sensitivity to specific plant traits would improve the accuracy of model predictions.

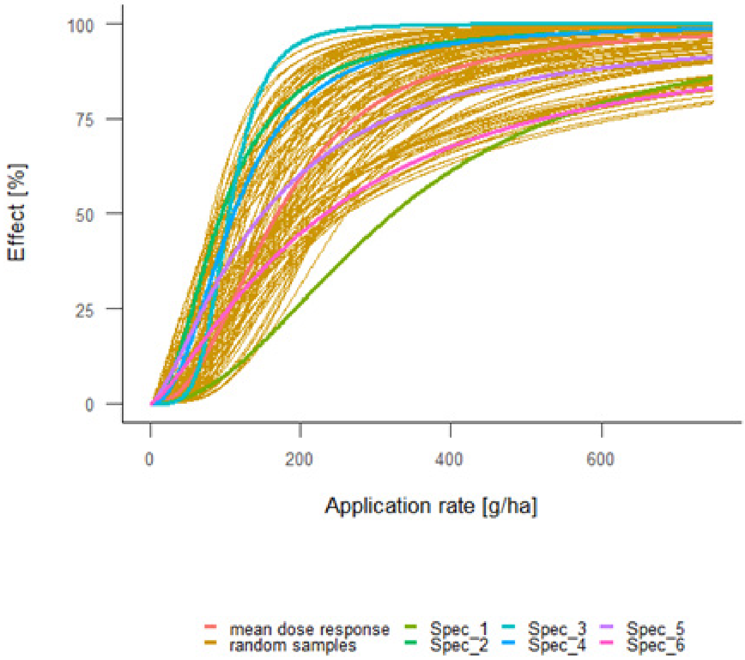

Figure 5.1: Estimated dose-responses for the 6 test species in Reuter and Siemoneit-Gast (2007) for the broad spectrum herbicide RoundUp®, the calculated mean dose response and 50 random dose responses based on the mean dose response and its standard deviation. The random dose responses are within the range of the species specific dose responses and thus cover the range of potential dose responses.

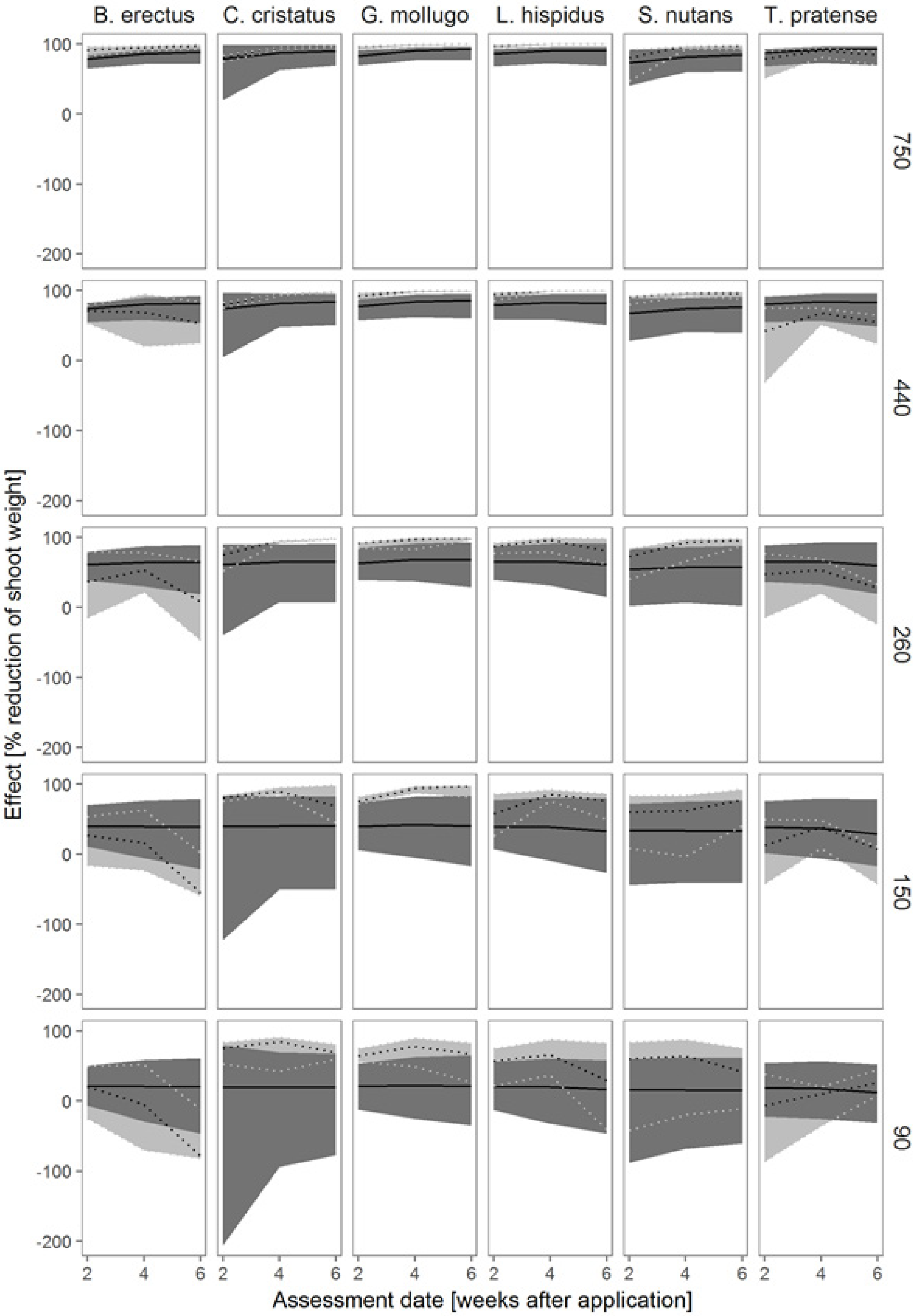

Figure 5.2: Model predictions for the effects on aboveground biomass on artificial communities similar to the study design of Reuter and Siemoneit-Gast (2007) for all tested application rates for the broad spectrum herbicide RoundUp® in mL/ha). Dose responses were assigned randomly and not species specific as in Reeg et al. (2018b). Black solid lines represent the median of the model predictions and dark gray ribbons show the upper and lower 2.5th percentile of the predictions. Dotted black lines show the empirically measured median and gray ribbons and dotted gray lines the upper and lower 2.5th percentile of these. The lowest rates tested were in the same range than the rates that would be applicable to the risk assessment considering European standard drift rates.

5.5 Ecological models and risk assessors: The hesitation of using models and how to build confidence in models

In general, risk assessors and risk managers are not trained in ecological modelling. They are used to assessing the risk based on the experimental studies (OECD 2006a, 2006b). They are often afraid that ecological models do not reflect the reality and thus mistrust model results. However, also the currently used greenhouse experiments do not reflect realistic field conditions and thus, assessment factors are used to cover for the uncertainties. Therefore, it is essential to provide a clear understanding about the model, including its fundamental assumptions, processes and functions; giving regulators or applicants of the model a clear idea of the models' possibilities and capabilities but also on possible limitations that need to be accounted for. In ecology, but also in ecotoxicology there is a great movement to develop suitable guidelines to document and describe ecological models (EFSA PPR Panel, 2014b; Grimm et al., 2014, 2010). All guidelines aim at facilitating the communication of ecological models and their development and testing. They include a description of the models purpose, fundamental processes, functions and underlying mechanisms of the model, data input needed to use the model; but they include also uncertainties or limitations of the model. To estimate the uncertainties of a model and to strengthen the credibility of a model a sensitivity analyses and a model validation with empirical data is essential (Augusiak et al., 2014).

In the case of IBC-grass, which I used in this thesis, there is well-developed documentation using the ODD protocol, a sensitivity analyses and a model validation for the basic model version (Weiß et al., 2014). In my thesis, I updated the ODD protocol including the processes of herbicide impact. The second chapter includes a short-term model validation and the third chapter a sensitivity analyses for the potentially affected plant attributes. Although these points already create a clear understanding of the model and its credibility, a long-term validation would build even stronger confidence in the model predictions. However, there are not only very few long-term field studies investigating the impacts of herbicide drift on non-target terrestrial plant communities (de Snoo and van der Poll, 1999; Kleijn and Snoeijing, 1997; Marrs and Frost, 1997; Schmitz et al., 2014), but also the data collection of these studies is in many cases insufficient for model validation. As a model validation needs a clear distinction of data used for model parameterization and for the actual validation, the data collection is often too small. However, Strandberg et al. (2012) established a field experiment in 2001, which they regularly sprayed with Glyphosate once a year since then. This data set seems promising to be used for a long-term validation of IBC-grass.

Besides the clear documentation of an ecological model and a sufficient reliability on the model predictions, the model should be easy to use and come with a manual describing the work-flow required for using the model in all detail, including the settings of the computing environment under which the model was developed and tested. A graphical user interface can facilitate the application of a model as it gives graphical guidance for parameter settings and the analyses of the output. The user manual should enable users not trained in ecological modelling to use the model. Currently, I am developing a graphical user interface for the IBC-grass model to facilitate the use in herbicide risk assessments. The package will include a Good Modelling Practice document, an ODD protocol and a user manual.

5.6 Other legislative directives to protect non-target terrestrial plants

Non-target organisms such as terrestrial plants are not only protected by assessing the impact of herbicide application on non-target organisms (Regulation 1107/2009 and Regulation 547/2011; (EC, 2009a, 2011)), but also by other directives such as the sustainable use directive, integrated weed management or other mitigation measures like buffer zones or compensation areas (Regulation 1107/2009 (EC, 2009a) and Regulation 547/2011 (EC, 2011), Directives 2009/128 (EC, 2009b), 2009/127 (EC, 2009c), 2000/60 (EC, 2013a) and 92/43 (EC, 1992), CAP (EC, 2013b)). Integrated weed management reduces the dependency on the use of chemicals by combining management strategies and scientific knowledge. For example, integrated weed management considers crop rotations, soil and cultivation practices and/or alternative weed control mechanisms over chemical weed control to support biodiversity in agricultural landscape.

Germany, for example, developed national action plans for the sustainable use of plant protection products (PPPs), e.g. to reduce the use of PPPs. One overarching goal is a 30 % reduction of environmental risk by reducing the exposure of non-target organisms. Placing modern pesticide application measures on the market, such as drift mitigation nozzles, reduces not only the herbicide drift to off-field areas, but also the amount of herbicide application (EC, 2009b, 2009c). In addition, non-sprayed areas can be established in field margins to mitigate the risk for non-target organisms (EC, 1992, 2013a; Haddaway et al., 2018). These field strips should serve as buffer between the crop field and the non-target areas. However, in Rhineland-Palatine and Berlin-Brandenburg, Germany, such field margins are often very narrow and make up large parts of the semi-natural habitat in the agricultural landscape (Hahn et al., 2014). Thus, they actually are the non-target area which must be protected to maintain biodiversity. Only if the field margins have a specific width, part of it may serve as a buffer strip in order to maintain the biological diversity of these semi-natural areas (Hahn et al., 2014).

In addition to buffer zones compensation areas can be integrated in the agricultural landscape to improve biological and structural diversity (EC, 2013b). In the CAP reform, farmers receive payments for integrating at least in 5% of their arable area such ecological focus areas (e.g. fallow land, margins or hedges). These structural elements such as hedgerows serve as habitat for other wildlife species such as birds or rabbits which are just passing the agricultural field (Hahn et al., 2014; Jeltsch et al., 2013). Improving the connectivity between vegetated patches also promotes seed dispersal between patches and meta-population dynamics. As seed dispersal maintains the seed bank it can also buffer or diminish potential impacts on seed production.

One advantage of the approach presented in chapter 4 of my thesis is the possibility of testing different exposure rates. By predicting different exposure levels in the landscape using herbicide exposure models (e.g. Xplicit (Schad, 2013; Schad and Schulz, 2011)), the impact on plant communities can be predicted in different distances to the crop field. This method can serve as a link between the different directives. When this approach is combined with landscape models, e.g., it can be estimated how many compensation areas are needed to protect biological diversity in the landscape.

5.7 Conclusion and future perspectives

The importance of ecological models in risk assessment is constantly increasing. For example, herbicide exposure models are already frequently used to estimate residues in the landscapes (e.g. FOCUS DG SANTE (EC, 2018)) and TKTD models are included in the guidance document for non-target aquatic organisms as higher tier options (Ockleford et al., 2018). Furthermore, EFSA has launched the MUST-B project to develop a model for the risk assessment of bees (EFSA, 2016). However, for non-target terrestrial plants new guidelines are still under development. My thesis tackled main uncertainties mentioned by EFSA (2010, 2014a) in the current risk assessment of non-target terrestrial plants. As supported by the EFSA, I chose a trait-based modelling approach to estimate impact on plant community-level. This approach can predict the risk for non-target terrestrial plants based on SPGs, but it can also support the decision on which endpoint the risk assessment should be based upon and thus the endpoint-specific importance for the maintenance of the plant community structure and dynamic. I validated this modelling approach for short-term effects; however, a long-term validation will increase the credibility. Therefore, long-term field studies are required to collect the data necessary for model calibration and validation. Furthermore, the assignment of random dose-responses to the PFTs seems to be an appropriate work around. Empirical studies testing the correlation of herbicide effect with specific plant traits can improve the models' accuracy.

Especially as field studies are limited in time and space and having in mind the problem of standardization and reproducibility, IBC-grass represents a promising alternative to extrapolate empirical individual-level effects to community level risk assessments. In summary, the modelling approach presented in my thesis can be a suitable higher tier option in future risk assessments of non-target terrestrial plants. The acceptance of ecological models in risk assessments is constantly increasing, but it remains to be seen whether the new guidance document for non-target terrestrial plants will follow this direction and include ecological modelling as higher tier options.

6 References

Aavik T, Augenstein I, Bailey D, Herzog F, Zobel M, Liira J. 2008. What is the role of local landscape structure in the vegetation composition of field boundaries? Appl. Veg. Sci. 11, 375–386. doi:10.3170/2008-7-18486

Aerts R. 1999. Interspecific competition in natural plant communities: mechanisms, trade-offs and plant-soil feedbacks. J. Exp. Bot. 50, 29–37, http://dx.doi.org/10.1093/jexbot/50.330.29.

Andreasen C, Streibig JC. 2011. Evaluation of changes in weed flora in arable fields of Nordic countries - based on Danish long-term surveys. Weed Res. 51, 214–226. doi:10.1111/j.1365-3180.2010.00836.x

Arts GHP, Kohlschmid E, Maltby L, Mayer C, Meregalli G, Poulsen V, Streissl F. 2017. An ecosystem services approach to pesticide risk assessment and risk management of non-target terrestrial plants: recommendations from a 2nd SETAC Europe workshop. Society of Environmental Toxicology and Chemistry (SETAC), November 2017

Augusiak J, Van den Brink PJ, Grimm V. 2014. Merging validation and evaluation of ecological models to "evaludation": A review of terminology and a practical approach. Ecol. Modell. 280. doi:10.1016/j.ecolmodel.2013.11.009

Bagg J, Ball B, Banks S, Baute T, Bohner H, Brown C, Cowbrough M, Dyck J, Ferguson T, Follings J, Hall B, Hayes A, Johnson P, Kyle J, McDonald I, Moran M, Munroe J, Quesnel G, Rabe N, Rosser B, Spieser H, Stewart G, Tenuta A, Verhallen A. 2017. Weed control. In Brown C, Follings J, Moran M, Rosser B, eds, Agronomy Guide for Field Crops. Publication 811. Ontario Ministry of Agriculture, Food and Rural Affairs, Delhi, Ontario, Canada, pp 273–291.

Baird DJ, Rubach MN, Van den Brink PJ. 2008. Trait-Based Ecological Risk Assessment (TERA): The New Frontier. Integr. Environ. Assess. Manag. 4, 2. doi:10.1897/IEAM_2007-063.1

Bakker JP, Poschlod P, Strykstra RJ, Bekker RM, Thompson K. 1996. Seed banks and seed dispersal: Important topics in restoration ecology. Acta Bot Neerl 45:461–490.

Barnthouse LW. 2004. Quantifying population recovery rates for ecological risk assessment. Environ Toxicol Chem 23:500–508.

Bell T, Freckleton RP, Lewis OT. 2006. Plant pathogens drive density dependent seedling mortality in a tropical tree. Ecol Lett 9:569–574.

Berger U, Piou C, Schiffers K, Grimm V. 2008. Competition among plants: Concepts, individual-based modelling approaches, and a proposal for a future research strategy. Perspect Plant Ecol Evol Syst 9:121–135.

Berryman AA. 1992. The Orgins and Evolution of Predator-Prey Theory. Ecology 73, 1530–1535. doi:10.2307/1940005

Bird SL, Perry SG, Ray SL, Teske ME. 2002. Evaluation of the AgDISP aerial spray algorithms in the AgDRIFT model. Environ. Toxicol. Chem. 21, 672, http://dx.doi.org/10.1897/1551-5028(2002)021<0672:EOTAAS>2.0.CO;2.

Boutin C, Rogers CA. 2000. Pattern of Sensitivity of Plant Species to Various Herbicides—An Analysis with Two Databases. Ecotoxicology 9, 255–272. doi:10.1023/A:1026518027350

Boutin C, Lee HB, Peart ET, Batchelor PS, Maguire RJ. 2000. Effects of the sulfonylurea herbicide metsulfuron methyl on growth and reproductuion of five wetland and terrestrial plant species. Environ Toxicol Chem 19:2532–2541.

Boutin C, Elmegaard N, Kjaer C. 2004. Toxicity testing of fifteen non-crops plants species with six herbicides in a greenhouse experiment: Implications for risk assessment. Ecotoxicology 13, 349–369.

Boutin C, Aya KL, Carpenter D, Thomas PJ, Rowland O. 2012. Phytotoxicity testing for herbicide regulation: shortcomings in relation to biodiversity and ecosystem services in agrarian systems. Sci. Total Environ. 415, 79–92, http://dx.doi.org/10.1016/j.scitotenv.2011.04.046.

Boutin C, Strandberg B, Carpenter D, Mathiassen SK, Thomas PJ. 2014. Herbicide impact on non-target plant reproduction: What are the toxicological and ecological implications? Environ Pollut 185:295–306.

Brook BW, O'Grady JJ, Chapman AP, Burgman MA, Akçakaya HR, Frankham R. 2000. Predictive accuracy of population viability analysis in conservation biology. Nature 404, 385–387. doi:10.1038/35006050

Buckelew LD, Pedigo LP, Mero HM, Owen MDK, Tylka GL. 2000. Effects of Weed Management Systems on Canopy Insects in Herbicide-Resistant Soybeans. J. Econ. Entomol. 93, 1437–1443. doi:10.1603/0022-0493-93.5.1437

Carpenter D, Boutin C. 2010. Sublethal effects of the herbicide glufosinate ammonium on crops and wild plants: Short-term effects compared to vegetative recovery and plant reproduction. Ecotoxicology 19:1322–1336.

Carpenter D, Boutin C, Allison JE. 2013. Effects of chlorimuron ethyl on terrestrial and wetland plants: Levels of, and time to recovery following sublethal exposure. Environ Pollut 172:275–282.

Caswell H. 2001. Matrix population models : construction, analysis, and interpretation. Sinauer Associates.

Christl H. 2015. Sensitivity of wild plant and crop species to plant protection products: literature review and analysis for SETAC AG Plants. SETAC Europe25th Annual Meeting in Barcelona, Spain.

Cousins SAO, Lavorel S, Davies I. 2003. Modeling the effects of landscape pattern and grazing regimes on the persistence of plant species with high conservation value in grasslands in south-eastern Sweden. Landsc Ecol 18:315–332. https ://doi.org/10.1023/A:10244 00913 488

Dalton RL, Boutin C. 2010. Comparison of the effects of glyphosate and atrazine herbicides on non-target plants grown singly and in microcosms. Environ.Toxicol. Chem. 29, 2304–2315, http://dx.doi.org/10.1002/etc.277.

Damgaard C, Strandberg B, Mathiassen SK, Kudsk P. 2011. The combined effect of nitrogen and glyphosate on the competitive growth, survival and establishment of Festuca ovina and Agrostis capillaris. Agric. Ecosyst. Environ.142, 374–381, http://dx.doi.org/10.1016/j.agee.2011.06.008.

Damgaard C, Strandberg B, Mathiassen SK, Kudsk P. 2014. The effect of glyphosate on the growth and competitive effect of perennial grass species in semi-natural grasslands. J. Environ. Sci. Health Part B 49, 897–908, http://dx.doi.org/10.1080/03601234.2014.951571.

DeAngelis DL, Mooij WM. 2005. Individual-based modeling of ecological and evolutionary processes. Annu Rev Ecol Evol Syst 36:147–168.

de Jong FMW, de Snoo GR, van de Zande JC. 2008. Estimated nationwide effects of pesticide spray drift on terrestrial habitats in the Netherlands. J Environ Manage 86:721–730. https://doi.org/10.1016/j.jenvman.2006.12.031

De Lange HJ, Lahr J, van der Poll JJC, Wessels Y, Faber JH. 2009. Ecological vulnerability in wildlife: An expert judgement and multicriteria analysis tool using ecological traits to assess relative impact of pollutants. Environ. Toxicol. Chem. 28, 2233. doi:10.1897/08-626.1

Denys C, Tscharntke T. 2002. Plant-insect communities and predator-prey ratios in field margin strips, adjacent crop fields, and fallows. Oecologia 130, 315–324. doi:10.1007/s004420100796

de Snoo GR. 1999. Unsprayed field margins: effects on environment, biodiversity and agricultural practice. Landsc. Urban Plann. 46, 151–160, http://dx.doi.org/10.1016/S0169-2046(99)00039-0.

de Snoo GR, van der Poll RJ. 1999. Effect of herbicide drift on adjacent boundary vegetation. Agric. Ecosyst. Environ. 73, 1–6, http://dx.doi.org/10.1016/S0167-8809(99)00008-0.

Díaz S, Cabido M. 2001. Vive la difference: Plant functional diversity matters to ecosystem processes. Trends Ecol Evol 16:646–655.

Dierschke H. 2004. Klassenübersicht der Molinion-Arrhenatheretea. In: Dierschke,H. (Ed.), Synopsis Der Pflanzengesellschaften Deutschlands. Heft 9. Selbstverlagder Floristisch-soziologischen Arbeitsgemeinschaft e.V., Göttingen, pp. 83–89.

Dierschke H, Waesch G, Fartmann T. 2004. Calthion palustris, in: Synopsis Der Pflanzengesellschaften Deutschlands Heft 9. pp. 10–16.

EC (European Commission). 1992. Council Directive 92/43/EEC of 21 May 1992 on the conservation of natural habitats and of wild fauna and flora. OJ L 206, 7.

EC (European Commission, Health & Consumer Protection Directorate-General (Directorate E—food safety, E1—plant health). 2002. Guidance Document on Terrestrial Ecotoxicology: Under Council Directive 91/414/EEC. Draft Work Doc SANCO/1032:1–39

EC (European Commission). 2009a. Regulation (EC) No 1107/2009 of the European Parliament and the council of 21 October 2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC. OJ L 309, 1.

EC (European Commission). 2009b. Directive 2009/128/EC of the European Parliament and of the Council of 21 October 2009, establishing a framework for Community action to achieve the sustainable use of pesticides. OJ L 309, 71.

EC (European Commission). 2009c. Directive 2009/127/EC of the European Parliament and of the Council of 21 October amending Directive 2006/42/EC with regard to machinery for pesticide application. OJ L 310, 29.

EC (European Commission). 2011. Commission Regulation (EU) No 547/2011 of 8 June 2011 implementing Regulation (EC) No 1107/2009 of the European Parliament and of the Council as regards labelling requirements for plant protection products. OJ L 155, 176.

EC (European Commission). 2013a. Directive 2013/39/EU of the European Parliament and of the Council of 12 August 2013 amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy. OJ L 226, 1.

EC (European Commission). 2013b. European Commission, "CAP Reform – an explanation of the main elements (MEMO/ 13/621)". European Commission, Brussels.

EC (European Commission). 2018. FOCUS DG SANTE [WWW Document]. URL https://esdac.jrc.ec.europa.eu/projects/focus-dg-sante

Ecobichon DJ. 2001. Pesticide use in developing countries. Toxicology 160, 27–33, http://dx.doi.org/10.1016/S0300-483X(00)00452-2.

EFSA (European Food Safety Authority). 2016. A mechanistic model to assess risks to honeybee colonies from exposure to pesticides under different scenarios of combined stressors and factors. EFSA Support. Publ. 13. doi:10.2903/sp.efsa.2016.EN-1069

EFSA PPR Panel (European Food Safety Authority, Panel on Plant Protection Products and Their Residues). 2009. Risk Assessment for Birds and Mammals. EFSA J. 7, 1438. doi:10.2903/j.efsa.2009.1438

EFSA PPR Panel (European Food Safety Authority, Panel on Plant Protection Products and Their Residues). 2010. Scientific opinion on the development of specific protection goal options for environmental risk assessment of pesticides, in particular in relation to the revision of the Guidance Documents on Aquatic and Terrestrial Ecotoxicology (SANCO/3268/2001 and SANCO/10329/2002). EFSA J 8:1821–1875.

EFSA PPR Panel (European Food Safety Authority, Panel on Plant Protection Products and Their Residues), 2013. Guidance on tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters. EFSA J. 11, 3290. doi:10.2903/j.efsa.2013.3290. Available

EFSA PPR Panel (European Food Safety Authority, Panel on Plant Protection Products and Their Residues). 2014a. Scientific opinion addressing the state of the science on risk assessment of plant protection products for non-target terrestrial plants. EFSA J 12.

EFSA PPR Panel (EFSA Panel on Plant Protection Products and their Residues), 2014b. Scientific Opinion on good modelling practice in the context of mechanistic effect models for risk assessment of plant protection products. EFSA J. 12, 3589–3591. doi:10.2903/j.efsa.2014.3589

EPPO (European and Mediterranean Plant Protection Organization). 2003. Environmental risk assessment scheme for plant protection products. EPPO Bull 33:195–209.

Eurostat, 2015. No Title [WWW Document]. URL https://ec.europa.eu/eurostat/statistics-explained/images/8/87/Land_cover%2C_2015.png

Everwand G, Fry EL, Eggers T, Manning P. 2014. Seasonal variation in the capacity for plant trait measures to predict grassland carbon and water fluxes. Ecosystems 17:1095–1108. https :// doi.org/10.1007/s10021-014-9779-z

Fischer A. 1985. Ruderale Wiesen – Ein Beitrag zur Kenntnis des Arrhenatherion-Verbandes. In: Dierschke, H. (Ed.), Tuexenia 5. Selbstverlag der Floristisch-soziologischen Arbeitsgemeinschaft e.V., Göttingen.

Fletcher JS, Pfleeger TG, Ratsch HC, Hayes R. 1996. Potential impact of low levels of Chlorsulfuron and other herbicides on growth and yield of nontarget plants. Environ Toxicol 15:1189–1196

Free JB. 1993. Insect pollination of crops. Academic Press.

Fry EL, Power SA, Manning P. 2014. Trait-based classification and manipulation of plant functional groups for biodiversity-ecosystem function experiments. J Veg Sci 25:248–261. https :// doi.org/10.1111/jvs.12068

Ganzelmeier H. 1995. Studies on the Spray Drift of Plant Protection Products: Results of a Test Program Carried Out Throughout the Federal Republic of Germany.

Gotelli NJ, McCabe DJ. 2002. Species Co-Occurrence: A Meta-Analysis of J. M. Diamond's Assembly Rules Model. Ecology 83, 2091. doi:10.2307/3072040

Grime JP. 2001. Plant Strategies, Vegetation Processes, and Ecosystem Properties. John Wiley and Sons, Chichester.

Grimm V, Revilla E, Berger U, Jeltsch F, Mooij WM, Railsback SF, Thulke HH, Weiner J, Wiegand

T, DeAngelis DL. 2005. Pattern-oriented modeling of agent-based complex systems: lessons from ecology. Science 310:987–991. https ://doi.org/10.1126/scien ce.11166 81

Grimm V, Berger U, Bastiansen F, Eliassen S, Ginot V, Giske J, Goss-Custard J, Grand T, Heinz SK, Huse G, Huth A, Jepsen JU, Jørgensen C, Mooij WM, Müller B, Pe'er G, Piou C, Railsback SF, Robbins AM, Robbins MM, Rossmanith E, Rüger N, Strand E, Souissi S, Stillman RA, Vabø R, Visser U, DeAngelis DL. 2006. A standard protocol for describing individual-based and agent-based models. Ecol Model 198:115–126.

Grimm V, Berger U, DeAngelis DL, Polhill JG, Giske J, Railsback SF. 2010. The ODD protocol: A review and first update. Ecol Model 221:2760–2768.

Grimm V. Martin BT. 2013. Mechanistic effect modeling for ecological risk assessment: Where to go from here? Integr. Environ. Assess. Manag. 9, e58–e63. doi:10.1002/ieam.1423

Grimm V, Augusiak J, Focks A, Frank BM, Gabsi F, Johnston ASA, Liu C, Martin BT, Meli M, Radchuk V, Thorbek P, Railsback SF. 2014. Towards better modelling and decision support: Documenting model development, testing, and analysis using TRACE. Ecol. Modell. 280, 129–139. doi:10.1016/j.ecolmodel.2014.01.018

Gross N, Bagousse-Pinguet YL, Liancourt P, Berdugo M, Gotelli NJ, Maestre FT. 2017. Functional trait diversity maximizes ecosystem multifunctionality. Nat Ecol Evol 1, 0132 DOI:10.1038/s41559-017-0.

Haddaway NR, Brown C, Eales J, Eggers S, Josefsson J, Kronvang B, Randall NP, Uusi-Kämppä J. 2018. The multifunctional roles of vegetated strips around and within agricultural fields. Environ. Evid. 7, 14. doi:10.1186/s13750-018-0126-2

Hahn M, Lenhardt PP, Brühl CA. 2014. Characterization of field margins in intensified agro-ecosystems-why narrow margins should matter in terrestrial pesticide risk assessment and management. Integr. Environ. Assess. Manag. 10, 456–462. doi:10.1002/ieam.1535

Henry M, Becher MA, Osborne JL, Kennedy PJ, Aupinel P, Bretagnolle V, Brun F, Grimm V, Horn J, Requier F. 2017. Predictive systems models can help elucidate bee declines driven by multiple combined stressors. Apidologie 48, 328–339. doi:10.1007/s13592-016-0476-0

Hewitt AJ. 2002. The practical use of AgDRIFT® and other drift exposure models for aerial: ground and orchard spray applications. Australas. J. Ecotoxicol. 8, 7–19.

Hewitt AJ, Teske ME, Thistle HW. 2002. The development of the AgDRIFT model for arial application and fixed-wing aircraft. Australas. J. Ecotoxicol. 8, 3–6.

Hicker T. 1999. Plant functional types and community characteristics along environmental gradients on Öland's Great Alvar (Sweden). University of Lund, Sweden

Hommen U, Forbes V, Grimm V, Preuss TG, Thorbek P, Ducrot V. 2016. How to use mechanistic effect models in environmental risk assessment of pesticides: Case studies and recommendations from the SETAC workshop MODELINK. Integr. Environ. Assess. Manag. 12, 21–31. doi:10.1002/ieam.1704

Iman RL. 1999. Latin Hypercube Sampling. Encyclopedia of statistical science update, vol 3. John Wiley & Sons Ltd, New York, pp 408–411

Jeltsch F, Bonte D, Pe'er G, Reineking B, Leimgruber P, Balkenhol N, Schröder B, Buchmann CM, Mueller T, Blaum N, Zurell D, Böhning-Gaese K, Wiegand T, Eccard JA, Hofer H, Reeg J, Eggers U, Bauer S. 2013. Integrating movement ecology with biodiversity research - exploring new avenues to address spatiotemporal biodiversity dynamics. Mov. Ecol. 1, 6. doi:10.1186/2051-3933-1-6

Kattge J, Diaz S, Lavorel S, Prentice IC, Leadley P, Boenisch G. 2011. TRY—a global database of plant traits. Glob Chang Biol 17:2905–2935

Kleijn D, Snoeijing G. 1997. Field boundary vegetation and the effects of agrochemical drift: botanical change caused by low levels of herbicide and fertilizer. J. Appl. Ecol. 34, 1413–1425.

Kleijn D, Verbeek M. 2000. Factors affecting the species composition of arable field boundary vegetation. J. Appl. Ecol. 37, 256–266.

Kleyer M, Bekker RM, Knevel IC, Bakker JP, Thompson K, Sonnenschein M, Poschlod P, van Groenendael JM, Klimes L, Klimešová J, Klotz S, Rusch GM, Hermy M, Adriaens D, Boedeltje G, Bossuyt B, Dannemann A, Endels P, Götzenberger L, Hodgson JG, Jackel AK, Kühn I, Kunzmann D, Ozinga WA, Römermann C, Stadler M, Schlegelmilch J, Steendamm HJ, Tackenberg O, Wilmann B, Cornelissen JHC, Eriksson O, Garnier E, Peco B. 2008. The LEDA traitbase: A database of life-history traits of Northwest European flora. J Ecol 96:1266–1274.

Klimešová J, de Bello F. 2009. CLO-PLA: The database of clonal and bud bank traits of Central European flora. J Veg Sci 20:511–516.

Klotz W, Kühn S, Durka I. 2002. BIOLFLOR: Eine Datenbank zu biologisch-ökologischen Merkmalen der Gef€aßpflanzen in Deutschland. In Klotz W, Kühn S, Durka I, eds, Schriftenreihe Für Vegetationskunde 38. Bundesamt für Naturschutz, Bonn, Deutschland, pp 1–334.

Körner K, Pfestorf H, May F, Jeltsch F. 2014. Modelling the effect of belowground herbivory on grassland diversity. Ecol Model 273:79–85.

Lazzerini G, Camera A, Benedettelli S, Vazzana C. 2007. The Role of Field Margins in Agro-biodiversity Management at the Farm Level. Ital. J. Agron. 2, 127. doi:10.4081/ija.2007.127

Marrs RH, Williams CT, Frost AJ, Plant RA. 1989. Assessment of the effects of herbicide spray drift on a range of plant species of conservation interest. Environ. Pollut. 59, 71–86. doi:10.1016/0269-7491(89)90022-5

Marrs RH, Frost AJ, Plant RA, Lunnis P. 1993. Determination of buffer zones to protect seedlings of non-target plants from the effects of glyphosate spraydrift. Agric. Ecosyst. Environ. 45, 283–293, http://dx.doi.org/10.1016/0167-8809(93)90077-3.

Marrs RH, Frost AJ. 1997. A microcosm approach to the detection of the effects of herbicide spray drift in plant communities. J. Environ. Manag. 50, 369–388, http://dx.doi.org/10.1006/jema.1996.9984.

Marshall EJ, Moonen A. 2002. Field margins in northern Europe: their functions and interactions with agriculture. Agric. Ecosyst. Environ. 89, 5–21. doi:10.1016/S0167-8809(01)00315-2

May F, Grimm V, Jeltsch F. 2009. Reversed effects of grazing on plant diversity: The role of below-ground competition and size symmetry. Oikos 118:1830–1843.

Meehl GA, Covey C, Delworth T, Latif M, McAvaney B, Mitchell JFB, Stouffer RJ, Taylor KE. 2007. The WCRP CMIP3 Multimodel Dataset: A New Era in Climate Change Research. Bull. Am. Meteorol. Soc. 88, 1383–1394. doi:10.1175/BAMS-88-9-1383

Moreby S, Southway S. 1999. Influence of autumn applied herbicides on summer and autumn food available to birds in winter wheat fields in southern England. Agric. Ecosyst. Environ. 72, 285–297. doi:10.1016/S0167-8809(99)00007-9

Morrison J, Izquierdo J, Plaza EH, González-Andújar JL. 2017. The role of field margins in supporting wild bees in Mediterranean cereal agroecosystems: Which biotic and abiotic factors are important? Agric. Ecosyst. Environ. 247, 216–224. doi:10.1016/J.AGEE.2017.06.047

Nelder JA, Mead R. 1965. A simplex method for function minimization. Comput J 7:308–313. https ://doi.org/10.1093/comjn l/7.4.308

Ockleford C, Adriaanse P, Berny P, Brock T, Duquesne S, Grilli S, Hernandez-Jerez AF, Bennekou SH, Klein M, Kuhl T, Laskowski R, Machera K, Pelkonen O, Pieper S, Smith RH, Stemmer M, Sundh I, Tiktak A, Topping CJ, Wolterink G, Cedergreen N, Charles S, Focks A, Reed M, Arena M, Ippolito A, Byers H, Teodorovic I. 2018. Scientific Opinion on the state of the art of Toxicokinetic/Toxicodynamic (TKTD) effect models for regulatory risk assessment of pesticides for aquatic organisms. EFSA J. 16. doi:10.2903/j.efsa.2018.5377

OECD (Organisation for Economic Co-operation and Development). 2006a. Test No. 208: Terrestrial plant test: Seedling emergence and seedling growth test. OECD Guidelines for the Testing of Chemicals. Paris, France.

OECD (Organisation for Economic Co-operation and Development). 2006b. Test No. 227: Terrestrial plant test: Vegetative vigour test. OECD Guidelines for the Testing of Chemicals. Paris, France.

Olff H, Ritchie ME. 1998. Effects of herbivores on grassland plant diversity. Trends Ecol. Evol. 13, 261–265. doi:10.1016/S0169-5347(98)01364-0

Olszyk DM, Burdick CA, Pfleeger TG, Lee EH, Watrud LS. 2004. Assessing the Risks to Non-Target Terrestrial Plants from Herbicides. J. Agric. Meteorol. 60, 221–242.

Pfestorf H, Körner K, Sonnemann I, Wurst S, Jeltsch F. 2016. Coupling experimental data with individual-based modelling reveals differential effects of root herbivory on grassland plant co-existence along a resource gradient. J. Veg. Sci. 27, 269–282. doi:10.1111/jvs.12357

Pfleeger T, Blakeley-Smith M, King G, Lee EH, Plocher M, Olszyk D. 2012. The effects of glyphosate and aminopyralid on a multi-species plant field trial. Ecotoxicology 21:1771–1787. https ://doi.org/10.1007/s10646-012-0912-5

Pfleeger T, Blakeley-Smith M, Lee EH, King G, Plocher M, Olszyk D. 2014. Effects of single and multiple applications of glyphosate or aminopyralid on simple constructed plant communities. Environ Toxicol Chem 33:2368–2378. https ://doi.org/10.1002/etc.2686

Prather TS, DiTomaso JM, Holt JS. 2000. Herbicide resistance : Definition and management strategies. UCANR Publications.

Rastetter EB, Aber JD, Peters DPC, Burke IC. 2003. Using mechanistic models to scale ecological processes across space and time. Bioscience 53:68–76. https ://doi.org/10.1641/0006-3568(2003)053[0068:ummtse]2.0.co;2

Rautmann D, Streloke M, Winkler R. 2001. New basic drift values in the Authorization procedure for plant protection products. Mitteilungen aus der Biol. Bundesanstalt für Land- und Forstwirtschaft Berlin- Dahlem 383, 133–141. doi:10.1029/2009GC002587

Reeg J, Schad T, Preuss TG, Solga A, Körner K, Mihan C, Jeltsch F. 2017. Modelling direct and indirect effects of herbicides on non-target grassland communities. Ecol Model 348:44–55.

Reeg J, Heine S, Mihan C, Preuss TG, McGee S, Jeltsch F. 2018a. Potential impact of effects on reproductive attributes induced by herbicides on a plant community. Environ Toxicol Chem 37(6):1707–1722

Reeg J, Schad T, Preuss TG, Solga A, Körner K, Mihan C, Jeltsch F. 2018b. Simulation of herbicide impacts on a plant community: comparing model predictions of the plant community model IBC-grass to empirical data. Environmental Sciences Europe 30:44. https://doi.org/10.1186/s12302-018-0174-9

Reuter S, Siemoneit-Gast S. 2007. Entwicklung einer weiterführenden Methode zur Bewertung des Risikos für terrestrische Pflanzen durch Exposition mit Pflanzenschutzmitteln und ihren Wirkstoffen

Reynolds HL, Packer A, Bever JD, Clay K. 2003. Grassroots ecology: Plantmicrobe-soil interactions as drivers of plant community structure and dynamics. Ecology 84:2281–2291.

Riemens MM, Dueck T, Kempenaar C. 2008. Predicting sublethal effects of herbicides on terrestrial non-crop plant species in the field from greenhouse data. Environ Pollut 155:141–149.

Riemens MM, Dueck T, Kempenaar C, Lotz LAP, Kropff MJJ. 2009. Sublethal effects of herbicides on the biomass and seed production of terrestrial non-crop plant species, influenced by environment, development stage and assessment date. Environ Pollut 157:2306–2313.

Rodríguez-Pastor R, Luque-Larena JJ, Lambin X, Mougeot F. 2016. "Living on the edge": The role of field margins for common vole (Microtus arvalis) populations in recently colonised Mediterranean farmland. Agric. Ecosyst. Environ. 231, 206–217. doi:10.1016/J.AGEE.2016.06.041

Rotchés-Ribalta R, Boutin C, Blanco-Moreno JM, Carpenter D, Sans FX. 2015. Herbicide impact on the growth and reproduction of characteristic and rare arable weeds of winter cereal fields. Ecotoxicology 24:991–1003.

Rubach MN, Baird DJ, Van den Brink PJ. 2010. A new method for ranking mode-specific sensitivity of freshwater arthropods to insecticides and its relationship to biological traits. Environ. Toxicol. Chem. 29, 476–487, http://dx.doi.org/10.1002/etc.55.

Sanchez-Bayo F, Van den Brink PJ, Mann RM. 2012. Ecological Impacts of Toxic Chemicals. Bentham Science Publishers.

Schad T, Schulz R. 2011. Xplicit, a novel approach in probabilistic spatiotemporally explicit exposure and risk assessment for plant protection products. Integr. Environ. Assess. Manag. 7, 612–623, http://dx.doi.org/10.1002/ieam.205.

Schad T. 2013. Xplicit – A Modelling Framework for Ecological Risk Characterisation at Landscape-scales in Regulatory Risk Assessment and Risk Management of Plant Protection Products.

Schibalski A, Körner K, Maier M, Jeltsch F, Schröder B. 2018. Novel model coupling approach for resilience analysis of coastal plant communities. Ecol. Appl. 28, 1640–1654. doi:10.1002/eap.1758

Schippers P, Kropff M. 2001. Competition for light and nitrogen among grassland species: a simulation analysis. Funct. Ecol. 15, 155–164. doi:10.1046/j.1365-2435.2001.00509.x

Schippers P, van Groenendael JM, Vleeshouwers LM, Hunt R. 2001. Herbaceous plant strategies in disturbed habitats. Oikos 95:198–210.

Schippers P, Joenje W. 2002. Modelling the effect of fertiliser, mowing, disturbance and width on the biodiversity of plant communities of field boundaries. Agric. Ecosyst. Environ. 93, 351–365. doi:10.1016/S0167-8809(01)00339-5

Schmitz J, Schäfer K, Brühl CA. 2013. Agrochemicals in field margins - Assessing the impacts of herbicides, insecticides and fertilizer on the common buttercup (*Ranunculus acris*). Environ. Toxicol. Chem. 32, 1124–1131. doi:10.1002/etc.2138

Schmitz J, Hahn M, Brühl CA. 2014. Agrochemicals in field margins: An experimental field study to assess the impacts of pesticides and fertilizers on a natural plant community. Agri Ecosyst Environ 193:60–69.

Schmolke A, Thorbek P, DeAngelis DL, Grimm V. 2010. Ecological models supporting environmental decision making: a strategy for the future. Trends Ecol Evol 25:479–486

Schmolke A, Kapo KE, Rueda-Cediel P, Thorbek P, Brain R, Forbes V. 2017a. Developing population models: A systematic approach for pesticide risk assessment using herbaceous plants as an example. Sci. Total Environ. 599–600, 1929–1938. doi:10.1016/j.scitotenv.2017.05.116

Schmolke A, Brain R, Thorbek P, Perkins D, Forbes V. 2017b. Population modeling for pesticide risk assessment of threatened species-A case study of a terrestrial plant, Boltonia decurrens. Environ. Toxicol. Chem. 36, 480–491. doi:10.1002/etc.3576

Schmolke A, Brain R, Thorbek P, Perkins D, Forbes V. 2018. Assessing and mitigating simulated population-level effects of 3 herbicides to a threatened plant: Application of a species-specific population model of Boltonia decurrens. Environ. Toxicol. Chem. 37, 1545–1555. doi:10.1002/etc.4093

Scholten H, Van der Tol MWM. 1994. Towards a metrics for simulation model validation. In: Grasman J, van Straten G (eds) Predictability and nonlinear modelling in natural sciences and economics. Springer, Dordrecht

Shugart HH. 1989. The role of ecological models in long-term ecological studies. In Likens GE, ed, Long-Term Studies in Ecology. Springer Verlag, New York, NY, USA, pp 90–109.

Stoyan D, Wagner S. 2001. Estimating the fruit dispersion of anemochorous forest trees. Ecol Model 145:35–47.

Strandberg B, Mathiassen SK, Bruus M, Kjaer C, Damgaard C, Andersen HV, Bossi R, Løfstrøm P, Larsen SE, Bak J, Kudsk P. 2012. Pesticide Research No. 137: Effects of herbicides on non-target plants: How do effects in standard plant test relate to effects in natural habitats? Danish Ministry of the Environment. Copenhagen, Denmark.

Tälle M, Deák B, Poschlod P, Valkó O, Westerberg L, Milberg P. 2016. Grazing vs. mowing: A meta-analysis of biodiversity benefits for grassland management. Agric. Ecosyst. Environ. 222, 200–212. doi:10.1016/j.agee.2016.02.008

Teske ME, Bird SL, Esterly DM, Curbishley TB, Ray SL, Perry SG. 2002. AgDRIFT: a model for estimating near-field spray drift from arial applications. Environ. Toxicol. Chem. 21, 659–671, http://dx.doi.org/10.1017/CBO9781107415324.004.

Tscharntke T, Klein AM, Kruess A, Steffan-Dewenter I, Thies C. 2005. Landscape perspectives on agricultural intensification and biodiversity - ecosystem service management. Ecol. Lett. 8, 857–874. doi:10.1111/j.1461-0248.2005.00782.x

Turnbull LA, Crawley MJ, Rees M. 2000. Are plant populations seed-limited? A review of seed sowing experiments. Oikos 88, 225–238. doi:10.1034/j.1600-0706.2000.880201.x

USEPA (US Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention). 2012a. Seedling emergence and seedling growth. OCSPP 850.4100. Ecological Effects Test Guidelines. Washington, DC.

USEPA (Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention. 2012b. Vegetative vigor. OCSPP 850.4150. Ecological Effects Test Guidelines. Washington, DC.

USEPA (Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention). 2012c. Early seedling growth toxicity test. OCSPP 850.4230. Ecological Effects Test Guidelines. Washington, DC.

van der Werf HMG. 1996. Assessing the impact of pesticides on the environment. Agric. Ecosyst.

Environ. 60, 81–96, http://dx.doi.org/10.1016/S0167-8809(96)01096-1.

Wagner V, Nelson CR. 2014. Herbicides can negatively affect seed performance in native plants. Restor. Ecol. 22, 288–291, http://dx.doi.org/10.1111/rec.12089.

Wang M, Rautmann D. 2008. A simple probabilistic estimation of spray drift factors determining spray drift and development of a model. Environ. Toxicol.Chem. 27, 2008–2626.

Warren JM, Topping CJ. 1999. A space occupancy model for the vegetation succession that occurs on set-aside. Agric. Ecosyst. Environ. 72, 119–129. doi:10.1016/S0167-8809(98)00168-6

Warren JM, Topping CJ. 2004. A trait specific model of competition in a spatially structured plant community. Ecol. Modell. 180, 477–485. doi:10.1016/j.ecolmodel.2004.04.033

Weiß L, Pfestorf H, May F, Körner K, Boch S, Fischer M, Müller J, Prati D, Socher SA, Jeltsch F. 2014. Grazing response patterns indicate isolation of semi-natural European grasslands. Oikos 123:599–612.

Weiß L. 2017. Understanding the emergence and maintenance of biodiversity in grasslands: linking individual plant responses to community patterns (Doctoral dissertation). University of Potsdam, Germany.

Wiegand T, Jeltsch F, Hanski I, Grimm V. 2003. Using pattern-oriented modeling for revealing hidden information: a key for reconciling ecological theory and application. Oikos 100:209–222. https ://doi.org/10.1034/j.1600-0706.2003.12027 .x

Wilson C, Tisdell C. 2001. Why farmers continue to use pesticides despite environmental, health and sustainability costs. Ecol. Econ. 39, 449–462, http://dx.doi.org/10.1016/S0921-8009(01)00238-5.

7 Supplemental material

7.1 Supplemental material of chapter 2

7.1.1 Model settings and parameters

Table 7.1: Parameters for the environmental settings

Variable	Explanation	Unit	Value
Plot size		cm	7x7; 20x20
Aboveground resources		resource units/cm^2	50-100
Belowground resources		resource units/cm^2	60-120
Grazing	Grazing probability		0
Trampling	Trampling probability		0
Cutting	Cutting events		0
Tmax	Maximal time simulated	year	1
Seed input		Nb of seeds/year	0
pbase	Base mortality	%	0

Table 7.2:PFT specific parameters

Variable	Explanation	Unit	PFT/species					
			B. erectus	*C. cristatus*	*G. mollugo*	*L. hispidus*	*S. nutans*	*T. pratense*
f_{leaf}	Growth form		0.75	0.75	1	0.5	0.75	0.75
m_{max}	Maximal plant mass	mg dry weight	5000	5000	2000	2000	2000	2000
m_{seed}	Seed mass	mg dry weight	1	1	0.3	0.3	0.3	0.3
$mean_{disp}$	Mean dispersal distance	m	0.1	0.1	0.3	0.3	0.3	0.3
std_{disp}	Standard deviation of dispersal distance	m	0.1	0.1	0.3	0.3	0.3	0.3
G_{max}	Maximal resource utilization per time step and ZOI area (equal for shoot and root)	resource units/ cm²	20	40	60	40	40	60
$surv_{max}$	Maximal survival time during resource stress	weeks	6	4	2	4	4	2
palatability	Susceptibility towards grazing		1	0.25	0.5	1	0.5	1
c_{shoot}	Above-ground ZOI area per leaf mass	cm²/ mg	1	0.5	0.75	1	0.75	1
RAR	Belowground ZOI area per root mass	cm²/ mg	1	1	1	1	1	1
growth	Conversion rate resource to biomass	mg/ resource unit	0.25					
mThres	Threshold of Δ_resmax for resource stress		0.2					
Resshare	Resource sharing between ramets of the same individual		0					
SpacerL	Spacer length	cm	0					
stdSpacerL	Standard deviation of spacer length	cm	0					
mSpacer	resources for 1 cm spacer (default=70)	resource unit/ cm	0					
Alloc_ root	Factor for increased allocation into roots		1	1	1	1	0.5	1
Alloc_ shoot	Factor for increased allocation into shoots		1	1	1	1	1	0.2

7.1.2 Repetition of the experimental monoculture control scenario

Since the model IBC-grass calculates plant growth based on the dry weight but Reuter and Siemoneit-Gast measured only fresh weight, we repeated the monoculture control scenario in order to calculate a dry to fresh weight ratio per plant species which we could then apply to all experimental data. The study was conducted in the greenhouse of the Botanical Garden in Potsdam, Germany, from March to May 2017.

SEEDLING CULTIVATION

The six plant species were cultivated on palettes with 240 cells (2.3x2.3x3.7 cm). The cells were filled with standard cultivation soil. At the beginning, several seeds were sown per cell to guarantee that at least one seed per cell germinated. If more than one seed germinated, all except for the one most in the middle were removed after emergence. After seeding, the palettes were put on a seed culture pot of 53x31x5.5 cm with a standard irrigation mat at the bottom of the pot. After initial watering from below to water the fleece mat, the palettes were watered on demand from above. At the beginning, a cold frame fleece was put on top of the palettes in order to support germination. It was removed during the main germination period. For each plant species, we seeded 160 cells, with the goal to have at least 120 emerging individuals, leading to 10 replicates per assessment date (3 assessment dates, 4 individuals per pot).

CULTURE CONDITIONS

When most seedlings reached the two to four leaf stage (BBCH 12-14), plant individuals were transplanted to the monoculture set up: 4 plant individuals of similar height were transplanted (homogenously distributed) into one pot (7x7x5 cm, filled with medium loamy soil and a deposit fertilizer). Plants were watered from above on demand.

The emergence rate differed strongly between the plant species. E.g. for *Bromus erectus* very few individuals emerged. Thus, the number of pots/replicates per species was different (Table 7.3).

Table 7.3: Number of replicates per plant species after transplantation. One replication represents one pot with 4 individuals.

Assessment date	*B. erectus*	*C. cristatus*	*G. mollugo*	*L. hispidus*	*S. nutans*	*T. pratense*
2	3	10	9	4	8	8
4	3	10	9	4	8	9
6	4	10	9	4	8	9
Sum	10	30	27	12	24	26

MEASUREMENTS

Aboveground biomass was harvested from a fraction of the replicates 2, 4 and 6 weeks after transplantation (see Table 7.3). During the experiment, some plants died. Only pots with at least one living plant were included in the assessment. Pots with only dead plants were ignored and therefore, the number of replicates decreased for some plant species (namely *C. cristatus, L. hispidus* and *T. pratense,* see Tables 7.3 vs. 7.4). However, at least 3 pots/replicates were measured per assessment date and species. Fresh weight per pot was measured directly after harvesting (excluding dead plants). The plants were dried for 3 days at 60 degrees Celsius to measure the dry weight. Afterwards, the ratio of dry to fresh weight was calculated per pot/replicate.

RESULTS

The fresh to dry weight ratios are similar between the tested species except for *T. pratense,* which had the highest ratios (Table 7.4). We used the mean of all assessment dates as a factor to convert the fresh weight measured in the study of Reuter and Siemoneit-Gast (2007) to dry weight. Based on this conversion factor, the modelled monoculture control dry weights fit to the converted dry weights of the experimental monoculture controls in the study of Reuter and Siemoneit-Gast (2007) (see Figure 2.2).

Table 7.4: Mean dry to fresh weight ratios for the three assessment dates: 2, 4 and 6 weeks after transplantation. Numbers in brackets represent the number of replicates (i.e. the number of pots).

Assessment date	*B. erectus*	*C. cristatus*	*G. mollugo*	*L. hispidus*	*S. nutans*	*T. pratense*
2	27% (3)	21% (10)	18% (9)	21% (4)	17% (8)	20% (8)
4	26% (3)	33% (10)	26% (9)	16% (4)	21% (8)	52% (9)
6	23% (4)	25% (9)	24% (9)	16% (3)	20% (8)	32% (4)
Overall mean	25%	27%	22%	18%	19%	36%

7.1.3 Complete significance test results

Table 7.5: Welch Two Sample t-test statistics for the model calibration (using monoculture control data).

PFT	Time [week]	Value t-statistic	Degrees of freedom	estimate		p-value	
				model	experiment		
Bromus erectus	2	1.17	7	120.06	101.25	0.282	n.s.
	4	1.19	6	321.76	257.86	0.279	n.s.
	6	0.21	7	531.85	515.31	0.84	n.s.
Cynosurus cristatus	2	1.38	7	28.56	21.26	0.21	n.s.
	4	1.7	7	142.64	82.35	0.133	n.s.
	6	3.76	7	344.96	147.83	0.007	**
Galium mollugo	2	1.31	7	108.79	84.43	0.231	n.s.
	4	0.04	7	296.51	294.8	0.969	n.s.
	6	-1.14	7	452.38	492.25	0.291	n.s.
Leontodon hispidus	2	-0.6	7	141.78	163.58	0.565	n.s.
	4	-1.58	7	332.29	456.53	0.157	n.s.
	6	-3.27	7	442.54	592.2	0.014	*
Silene nutans	2	1.59	6	51.08	35.56	0.162	n.s.
	4	1.1	7	146.47	117.09	0.31	n.s.
	6	0.03	7	240.88	239.16	0.98	n.s.
Trifolium pratense	2	0.9	6	278.47	223.71	0.402	n.s.
	4	-0.22	7	432.22	449.55	0.831	n.s.
	6	-1.8	7	517.25	973.35	0.115	n.s.

Table 7.6: Welch Two Sample t-test statistics for the model prediction of community control growth

PFT	Time [week]	Value t-statistic	Degrees of freedom	estimate		p-value	
				model	experiment		
Bromus erectus	2	0.34	5	106.91	98.33	0.746	n.s.
	4	-0.91	5	187.27	224.58	0.403	n.s.
	6	0.27	5	251.18	242.92	0.8	n.s.
Cynosurus cristatus	2	4.68	5	105.08	40.05	0.005	**
	4	3.03	5	193	102.6	0.029	*
	6	2.16	5	281.72	177.75	0.083	n.s.
Galium mollugo	2	1.53	5	139.61	92.77	0.187	n.s.
	4	0.44	5	294.03	271.33	0.677	n.s.
	6	1.11	5	433.61	385.73	0.318	n.s.
Leontodon hispidus	2	0.09	5	187.02	182.4	0.931	n.s.
	4	-0.79	5	357.91	452.7	0.464	n.s.
	6	-1.04	5	450.22	531.9	0.345	n.s.
Silene nutans	2	1.47	5	84.4	52.88	0.203	n.s.
	4	1.91	5	136.15	90.57	0.115	n.s.
	6	1.28	5	178.91	137.75	0.256	n.s.
Trifolium pratense	2	-0.32	5	217.74	241.2	0.763	n.s.
	4	-1.01	5	458.37	726	0.357	n.s.
	6	-2.54	5	592.81	1318.2	0.052	n.s.

7.1.4 Dose response curves for all species and both herbicides

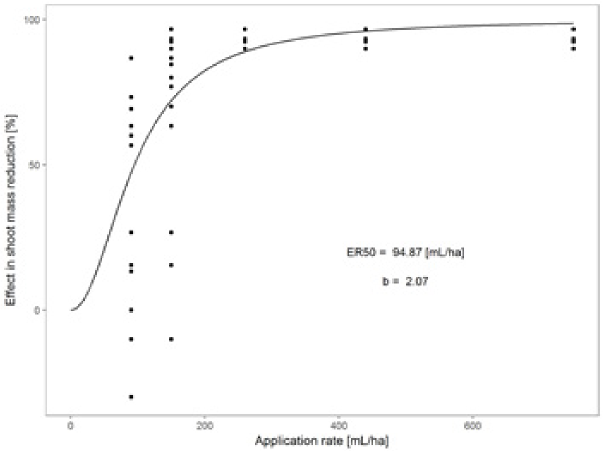

Figure 7.1: **Effects on the fresh weight (% reduction of fresh weight) of *C. cristatus* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the broad spectrum herbicide RoundUp®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

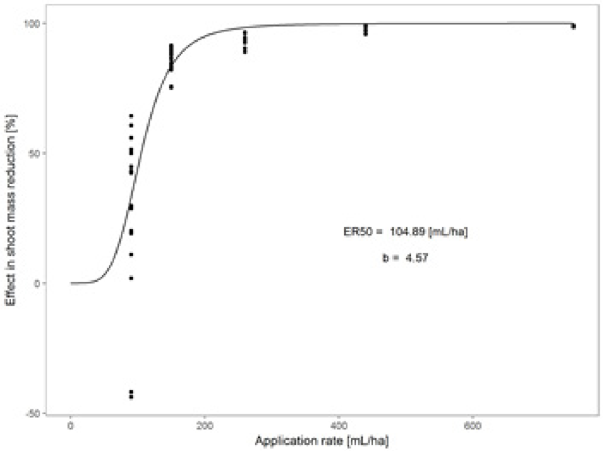

Figure 7.2: **Effects on the fresh weight (% reduction of fresh weight) of *G. mollugo* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the broad spectrum herbicide RoundUp®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

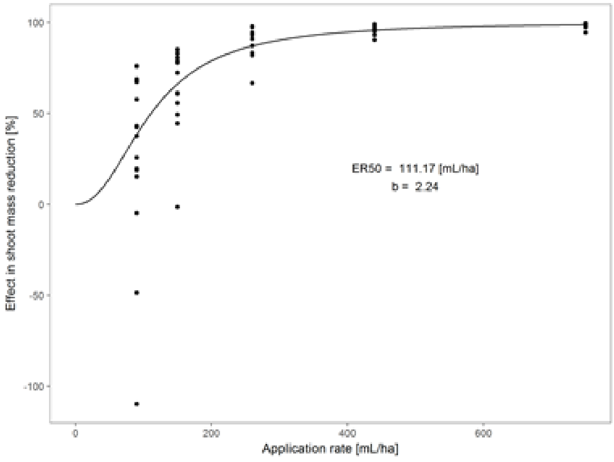

Figure 7.3: **Effects on the fresh weight (% reduction of fresh weight) of *L. hispidus* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the broad spectrum herbicide RoundUp®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

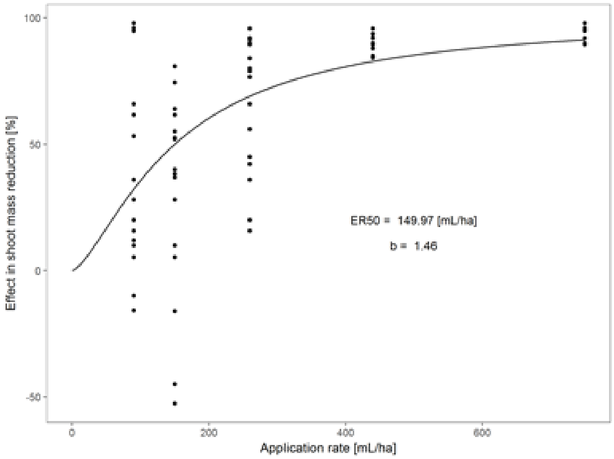

Figure 7.4: **Effects on the fresh weight (% reduction of fresh weight) of *S. nutans* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the broad spectrum herbicide RoundUp®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

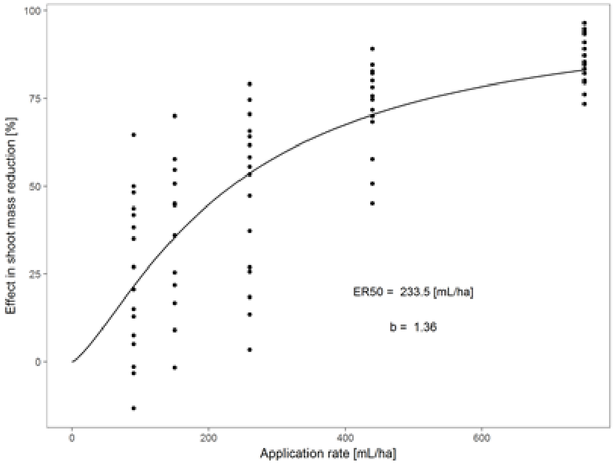

Figure 7.5: **Effects on the fresh weight (% reduction of fresh weight) of *T. pratense* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the broad spectrum herbicide RoundUp®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

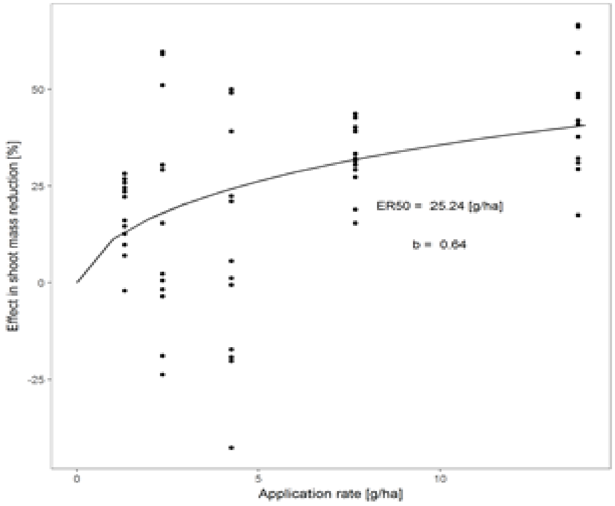

Figure 7.6: **Effects on the fresh weight (% reduction of fresh weight) of *B. erectus* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the selective herbicide Monitor®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

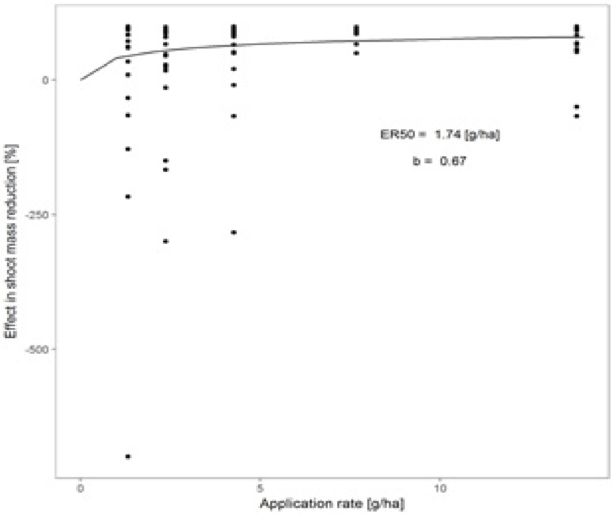

Figure 7.7: **Effects on the fresh weight (% reduction of fresh weight) of *C. cristatus* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the selective herbicide Monitor®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

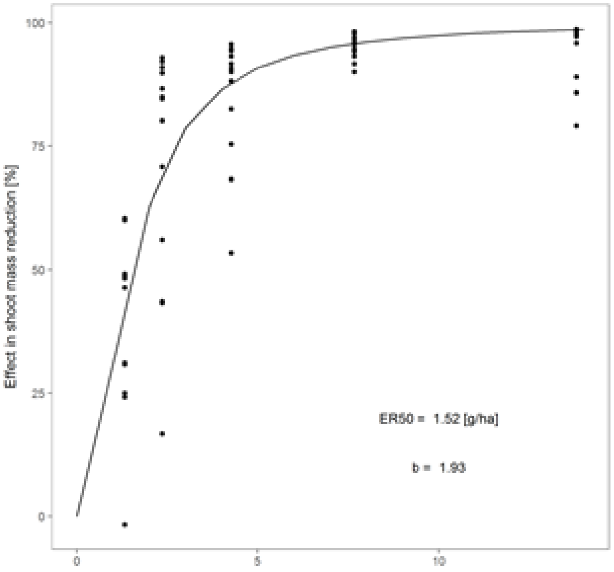

Figure 7.8: **Effects on the fresh weight (% reduction of fresh weight) of *G. mollugo* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the selective herbicide Monitor®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

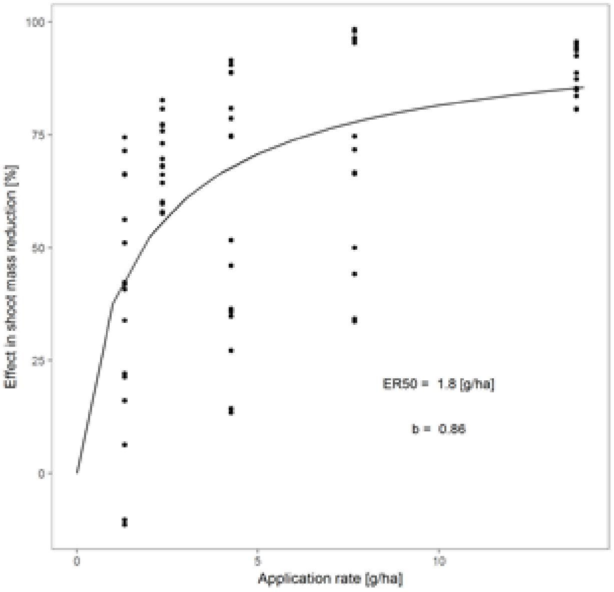

Figure 7.9: **Effects on the fresh weight (% reduction of fresh weight) of *L. hispidus* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the selective herbicide Monitor®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

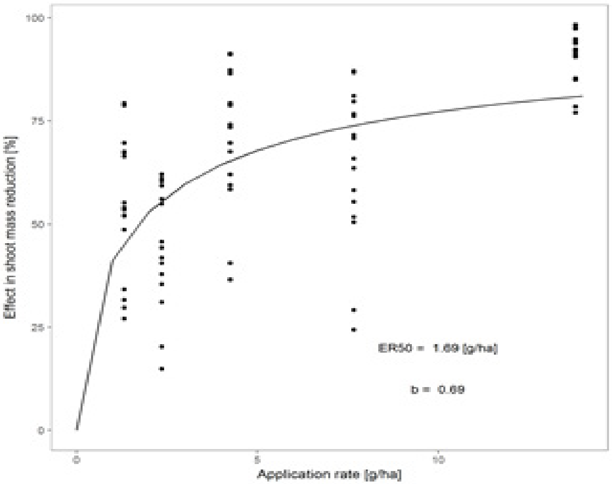

Figure 7.10: **Effects on the fresh weight (% reduction of fresh weight) of *S. nutans* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the selective herbicide Monitor®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

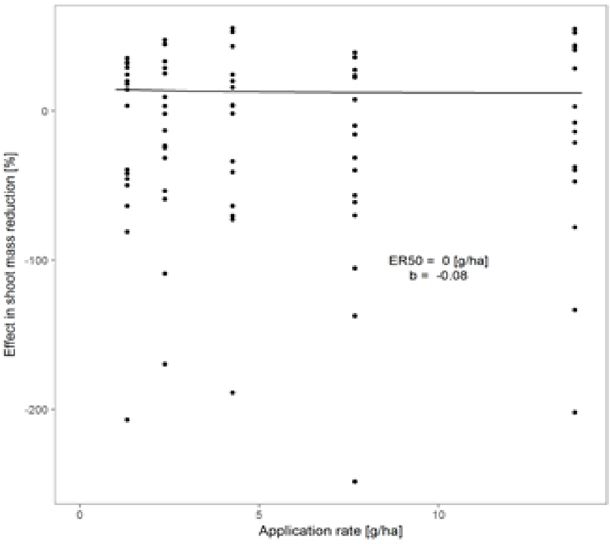

Figure 7.11: **Effects on the fresh weight (% reduction of fresh weight) of *T. pratense* in the monoculture treatment 4 weeks after application, when sprayed with different application rates of the selective herbicide Monitor®.** Points show the empirically measured data and the line the estimated dose response function, with the predictors for the ER50 value and the slope b.

7.1.5 Results for all application rates

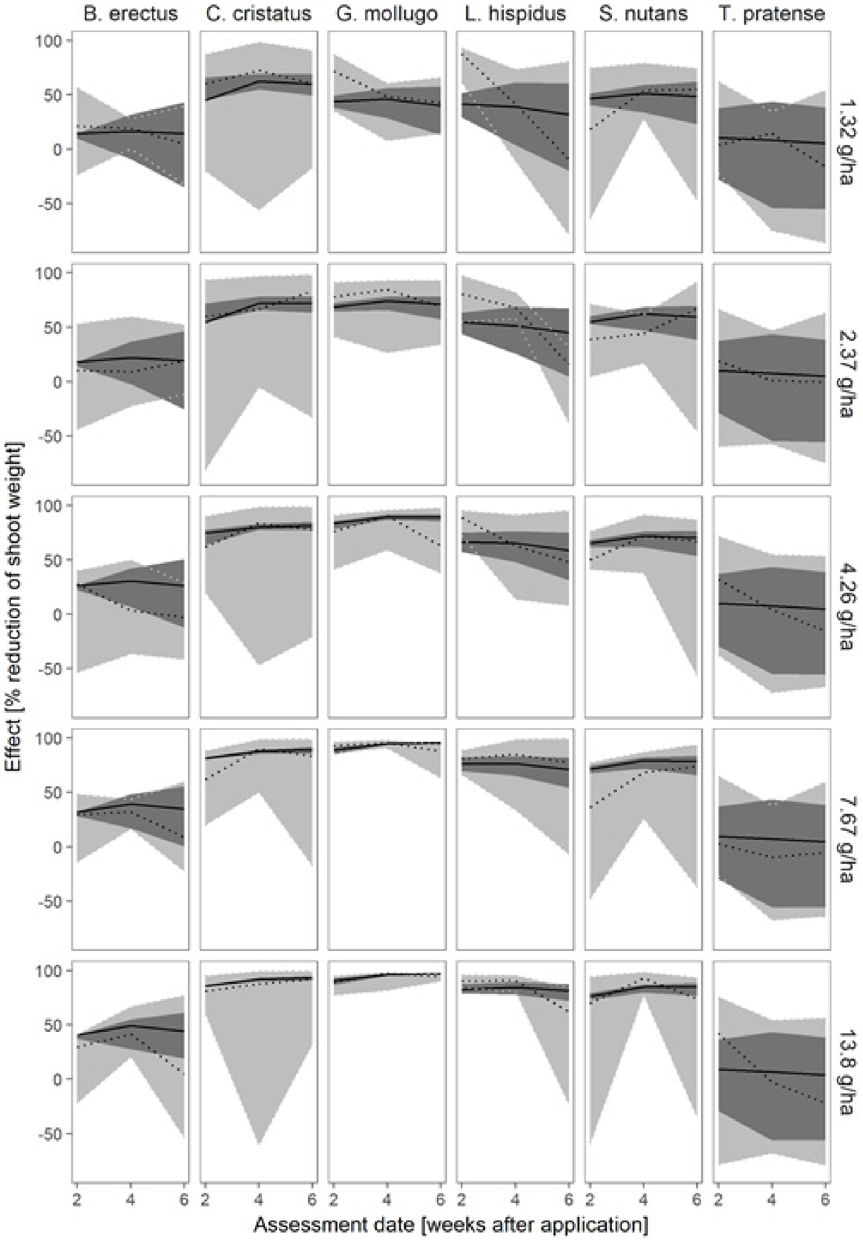

Figure 7.12: Effects on species specific shoot masses (treatment/control) in the monocultures after application of the selective herbicide Monitor®. Black solid lines represent the median of the model predictions and dark grey ribbons show the upper and lower 2.5th percentile of the predictions. Dotted black lines show the empirically measured median and grey ribbons and dotted grey lines the upper and lower 2.5th percentile of these.

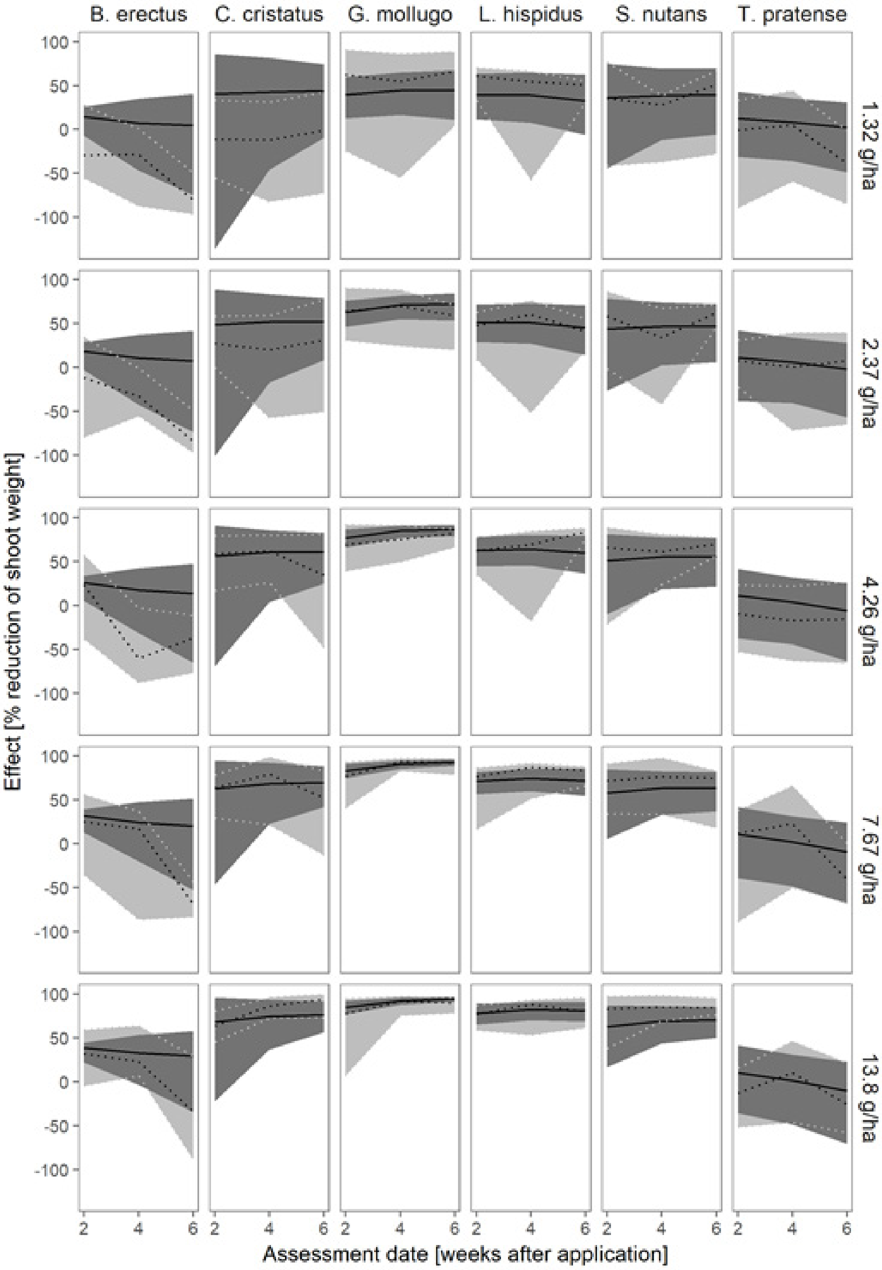

Figure 7.13: **Effects on species specific shoot masses (treatment/control) in the artificial communities after application of the selective herbicide Monitor®.** Black solid lines represent the median of the model predictions and dark grey ribbons show the upper and lower 2.5th percentile of the predictions. Dotted black lines show the empirically measured median and grey ribbons and dotted grey lines the upper and lower 2.5th percentile of these.

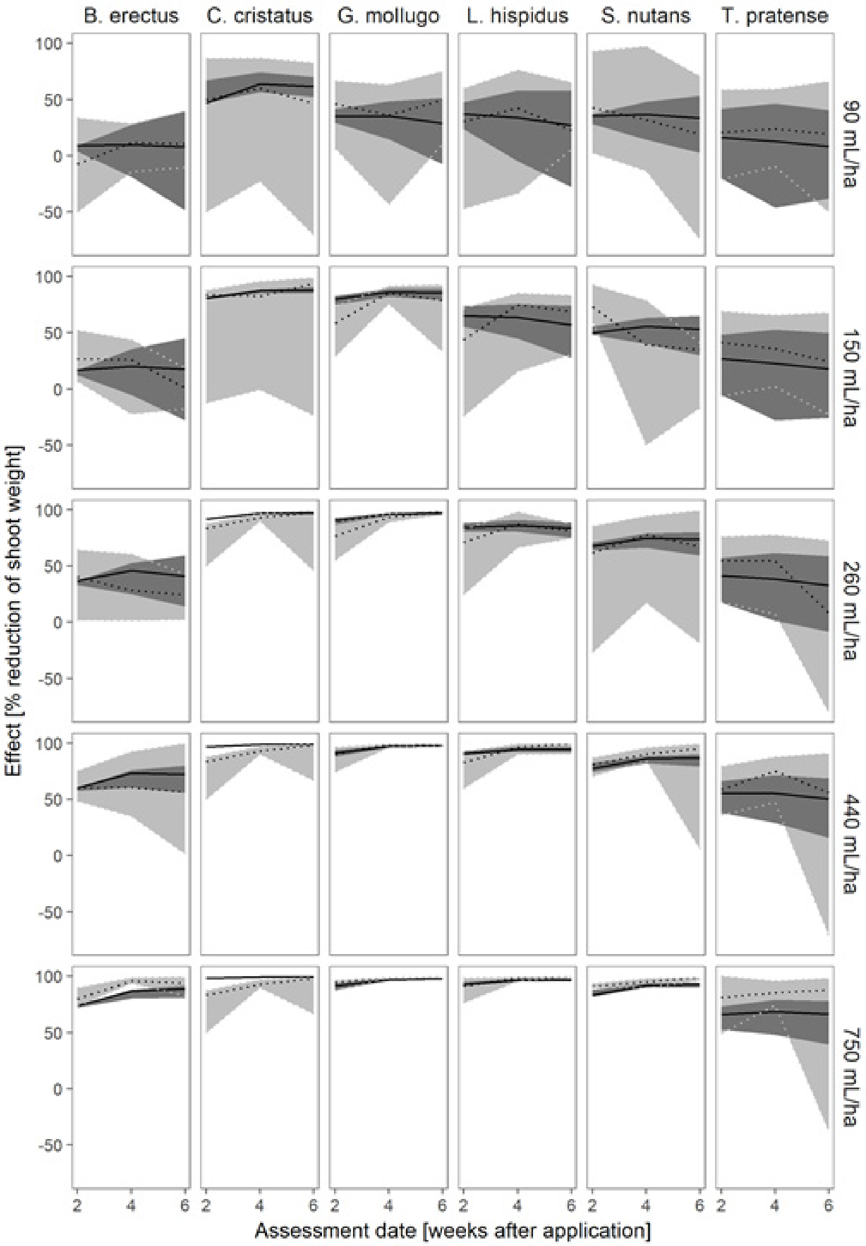

Figure 7.14: **Effects on species specific shoot masses (treatment/control) in the monocultures after application of the broad spectrum herbicide RoundUp®.** Black solid lines represent the median of the model predictions and dark grey ribbons show the upper and lower 2.5th percentile of the predictions. Dotted black lines show the empirically measured median and grey ribbons and dotted grey lines the upper and lower 2.5th percentile of these.

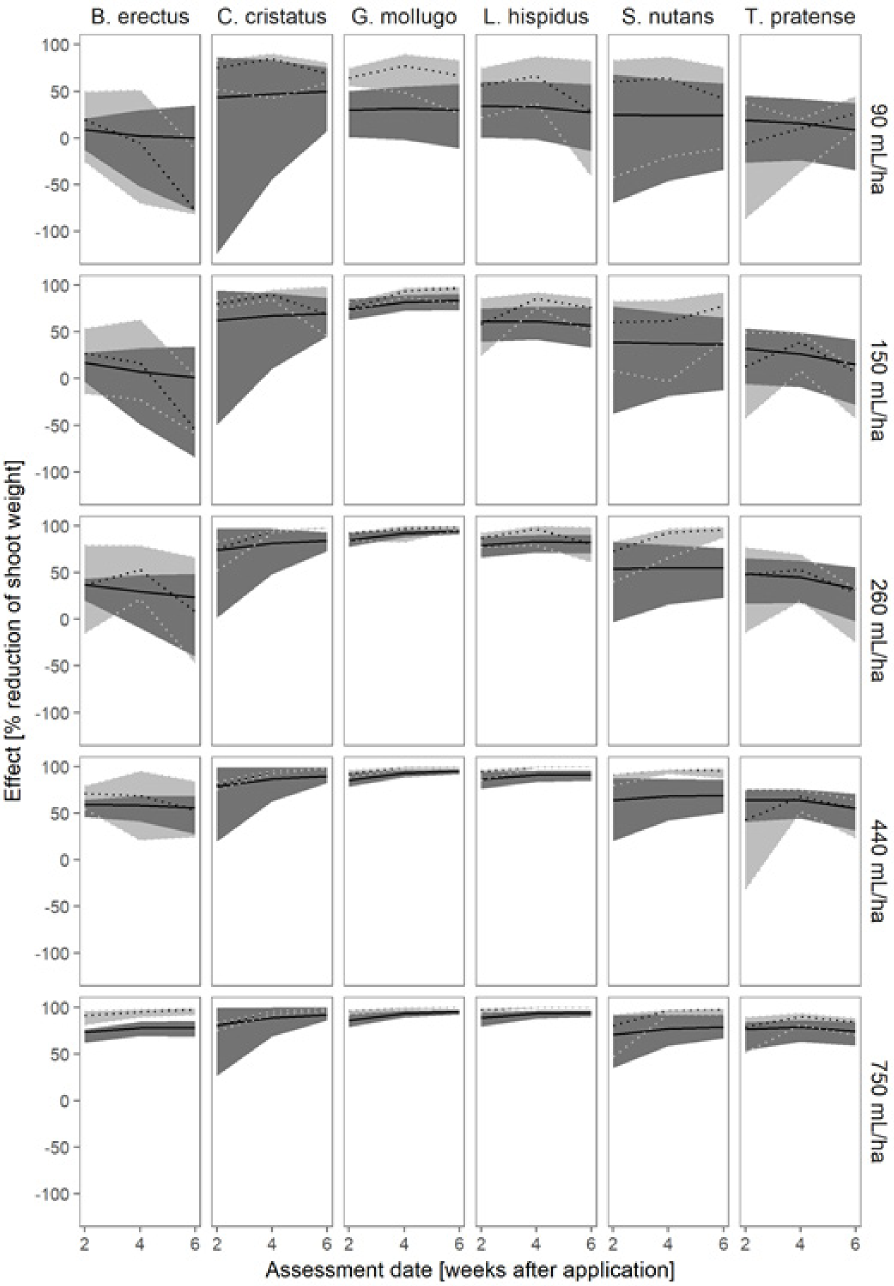

Figure 7.15: Effects on species specific shoot masses (treatment/control) in the artificial communities after application of the broad spectrum herbicide RoundUp®. Black solid lines represent the median of the model predictions and dark grey ribbons show the upper and lower 2.5th percentile of the predictions. Dotted black lines show the empirically measured median and grey ribbons and dotted grey lines the upper and lower 2.5th percentile of these.

7.1.6 Comparison of plant growth modelled in single pots, monocultures and in the empirical monoculture

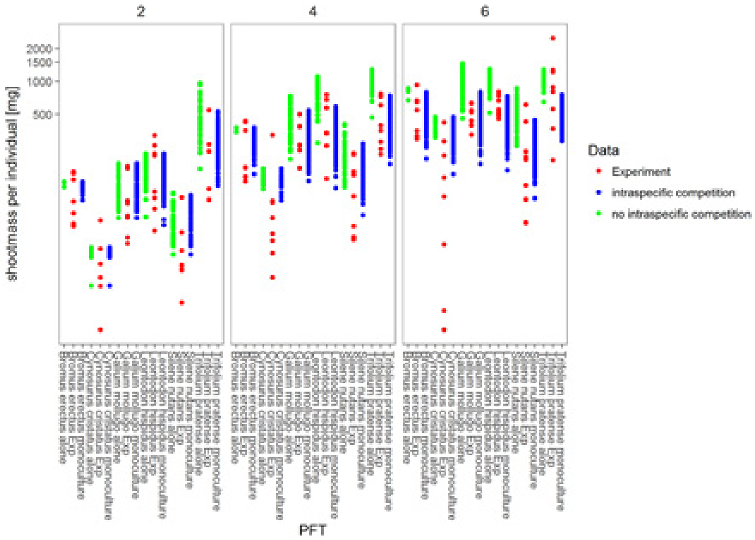

Figure 7.16: Simulated shoot masses for plant individuals grown in single pots (no intraspecific competition), in monocultures (intraspecific competition) vs. shoot masses measured in monoculture controls (Experiment).

7.2 Supplemental material of chapter 3

7.2.1 ODD-protocol

The model description follows the ODD (Overview, Design concepts, Details) protocol for describing individual- and agent-based models (Grimm et al., 2010, 2006). We based our simulation experiments on the grassland community model IBC-grass (Körner et al., 2014; May et al., 2009; Reeg et al. 2017; Weiss et al., 2014). This ODD-protocol is based on the version by Reeg et al. (2017), modified processes and extensions are marked in bold.

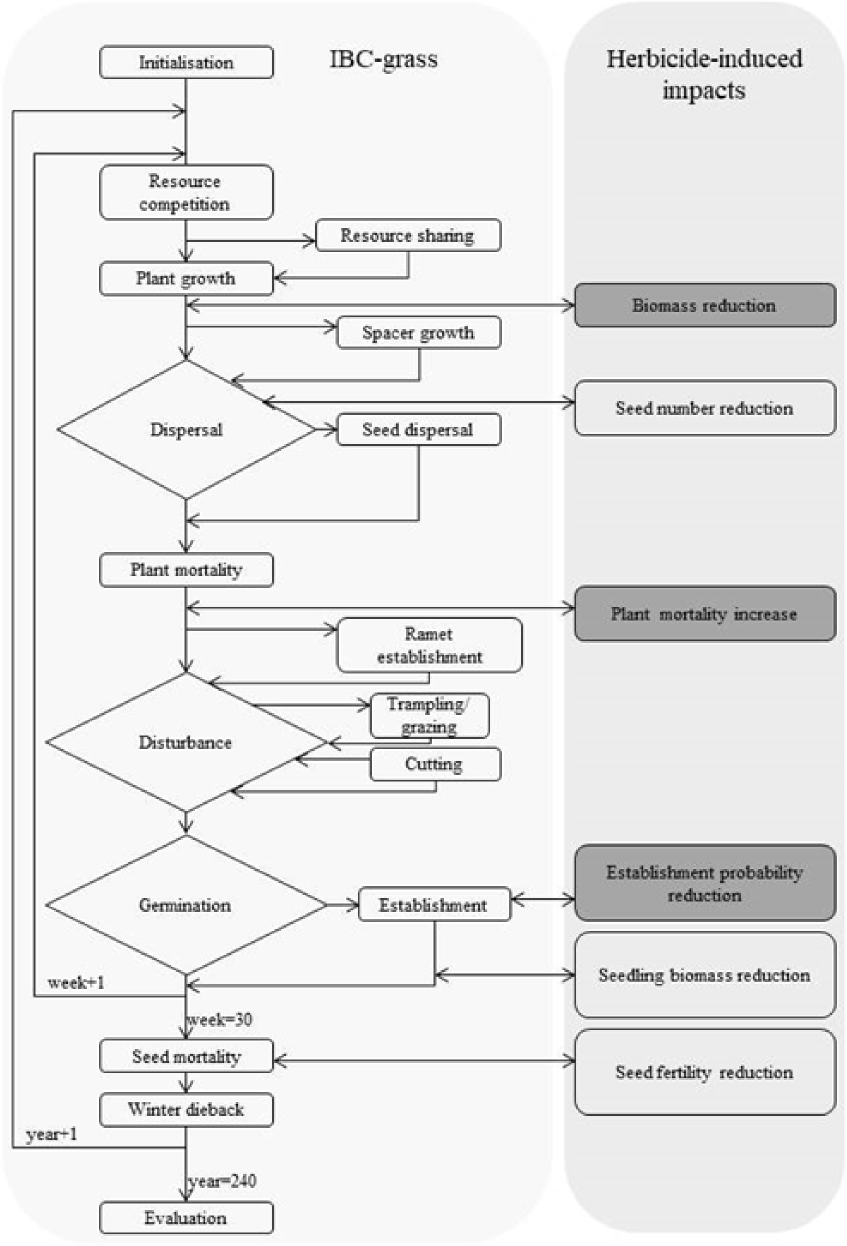

Figure 7.17: Flow chart of the processes within IBC-grass. Dark grey boxes mark plant attributes currently tested in ecotoxicological standard studies.

PURPOSE

This extended version of IBC-grass is designed to analyse potential on a local plant community adjacent to arable field effects induced by herbicide drift.

ENTITIES, STATE VARIABLES AND SCALES

The model simulates plant community processes within an approx. 3 m^2 patch designed as a grid of 173*173 grid cells, i.e. one grid cell represents 1cm^2. Each grid cell can comprise several seeds and not more than one individual plant. Each seed is described with the state variable of its specific location on the grid and moreover its age and mass. An individual plant can either be a ramet of a clonal plant type or a non-clonal plant. Each plant individual is described by its specific position on the grid, the duration of resource stress exposure, the shoot, root and reproductive mass and the presence of growing spacers in case of clonal plant types. Plant individuals are categorized into plant functional types (PFT), which differ in their characteristics of 12 selected trait parameters. Plant individuals have circular area around their stem, the 'zone-of-influence' (ZOI). Within this area, plants acquire and compete for resources in the case of overlapping ZOIs. Two compartments (layers) are distinguished: above- and belowground. ZOIs are determined by the specific above- and belowground biomasses of the individual plant. As plants grow, the ZOI areas increase over time. One simulated time step represents one week; in each year 30 weeks of vegetation period are simulated.

PROCESS OVERVIEW AND SCHEDULING

The schedule of the simulated processes is shown in Figure 7.17. All processes except for seed dispersal, seedling establishment and cutting are executed each week. Seed dispersal, seedling establishment and cutting are limited to certain weeks within the year. Winter dieback of aboveground biomass and seed mortality is considered once at the end of each year. The plant's functional traits determine all processes. The state variable mass and age are synchronously updated each week and year after all model entities have been processed.

DESIGN CONCEPTS

BASIC PRINCIPLES

The model simulates local competition by using the zone-of-influence approach in two layers: above ground and below ground. Thereby, it distinguishes between symmetric (below ground) and asymmetric (above ground) competition. Competition among individuals of the same functional type (i.e. intra-PFT competition) is assumed to be higher than competition between individuals of different PFTs (i.e. inter-PFT competition) (Berendse, 1983). In this model version, density-dependent mortality is introduced.

EMERGENCE

Endpoints on community level, e.g. PFT diversity and biomass, emerge from individual plant-plant interactions, resource levels, disturbance events like trampling, grazing and cutting and herbicide exposure effects.

ADAPTATION

Plants balance the uptake of above- and belowground resources by adapting the allocation of resources to shoot and root growth.

INTERACTIONS

Plants compete for resources and space by the ZOI approach.

STOCHASTICITY

Demographic noise is included by modelling seed dispersal, seedling establishment, seed mortality and plant mortality stochastically. In addition, grazing and trampling occur randomly on the simulated grid. The plant's individual probability to be grazed is determined by its specific plant traits.

INITIALIZATION

Initially, ten seeds per PFT of the regional PFT pool (see 7.2.2) were randomly distributed over the grid. Their germination probability was set to 100% in order to have equal initial population sizes of all PFTs. Above- as well as below ground resources are distributed spatially and temporally homogenous.

INPUT

The model needs the information about the available PFT pool and the trait characteristics of the respective PFTs. In addition, herbicide effects are introduced either via an http-interface, which hands over species effect distributions generated by the model Xplicit or via a .txt file which includes the effect per year per attribute (see sub-model "herbicide exposure effects").

SUB-MODELS

Most sub-models are adopted from the model version described by Weiß et al. (2014). New and modified sub-models are marked in bold.

COMPETITION

Following the ZOI approach, plants compete for resources in a circular area around their central location point. To relate plant mass to the area covered (A_{shoot}), the allometric relation by Weiner et al. (2001) is used.

$$A_{shoot} = c_{shoot} \cdot (f_{leaf} \cdot m_{shoot})^{2/3} \quad \text{Eq. (7.2.1)}$$

Where c_{shoot} is a constant ratio between leaf mass and ZOI area and mshoot is vegetative shoot mass. The factor fleaf is introduced to describe different shoot geometries and is defined as the ratio between photosynthetic active (leaf) and inactive (stem) tissue. Only the former is considered for the calculation of the ZOI size. These circular areas are projected onto a grid of discrete cells. Grid cells thus contain the information by which plants they are covered, so that resource competition can be calculated cell by cell. The resources within a cell are shared among plants according to their relative competition coefficients (β_i). The resource uptake (Δres) of plant i from a cell with resource availability (Res_{cell}) covered by n plants is thus calculated as

$$\Delta res_i = \frac{\beta_i}{\sum_{j=1}^{n} \beta_j} \cdot Res_{cell} \quad \text{Eq. (7.2.2)}$$

Calculating βi in different ways allows including different modes of competition, i.e. symmetric or asymmetric (Weiner et al., 2001). We assume that the relative competitive ability of a plant is correlated with its maximum growth rate in the absence of resource competition. Therefore β_i is proportional to maximum resource utilization per unit area covered (ru_{max}, see Sub-model "Plant growth and mortality"). In the case of size-symmetric competition, β_i simply equals rumax:

$$\beta_i = ru_{max} \quad \text{Eq. (7.2.3)}$$

In the case of partially size-asymmetric competition β_i is a function of plant mass and shoot geometry:

$$\beta_i = ru_{max} \cdot m_{shoot} \cdot f_{leaf}^{-1} \quad \text{Eq. (7.2.4)}$$

The inverse of f_{leaf} is used, because plants with a lower fraction of leaf tissue are considered to be higher and thus show a higher competitive ability by overtopping other plants. In this way, plants with equal ru_{max} receive equal amounts of resources from one unit of area irrespective of their mass or height in the case of size-symmetric competition, while larger and higher plants receive a higher share of resources in proportion to their shoot geometry in the case of partially asymmetric competition (Schwinning and Parsons, 1999; Weiner et al., 2001). The resource uptake of a plant within one week can then be determined by summing the results of Eq. (7.2.2) over all cells covered by the plant.

To include differences between intra- and interspecific competition, individuals of the same PFT are considered as con-specifics and those of different PFTs as hetero-specifics. The relative competitive ability β_i of one plant is then determined as a decreasing function of the number of plants belonging to the same PFT (n_{PFT}) and covering the same cell:

$$\beta_i = ru_{max} \cdot \frac{1}{\sqrt{n_{PFT}}} \qquad \text{Eq. (7.2.5)}$$

Eq. (7.2.5) is used for size-symmetric competition instead of Eq. (7.2.3). In the case of size asymmetry, plant mass and geometry are taken into consideration according to Eq. (7.2.4). This approach represents a situation where intra-PFT competition is increased relatively to inter-PFT competition and therefore implicitly includes niche differentiation of resource competition at the cell scale, which has been known as an important factor for species coexistence (Chesson, 2000; Silvertown, 2004).

Plant growth and mortality.

Plant growth only depends on the resources (Δres) that the plant acquired during the current time step. In the absence of competition, plants show sigmoid growth. Therefore the growth equation used by Weiner et al. (2001) was adapted to the description of plant geometry used here:

$$\Delta m = g \cdot \left(\Delta res - c_{shoot} \cdot f_{leaf}{}^{2/3} \cdot ru_{max} \cdot \frac{m_{shoot}{}^{2}}{m_{max}{}^{4/3}} \right) \qquad \text{Eq. (7.2.6)}$$

where g is a constant conversion rate between resource units and plant biomass and m_{max} is the maximum mass of shoot and root, respectively. In addition, the maximum amount of resources that is allocated to growth each week is limited by a maximum resource utilization rate given by ru_{max} [resource units/cm^2] multiplied by ZOI area [cm^2]. If Eq. (7.2.6) yields a negative result, Δm is set to zero and thus negative growth is prohibited. Lateral plant growth is simulated by considering clonality of plants (see Growth, dispersal and establishment of spacers of clonal plant types).

Growth of generative reproductive mass is restricted to the time between weeks 16 – 21. In this period, a constant fraction of the resources (5 % for all PFTs) is allocated to growth of reproductive mass (Schippers et al., 2001), and reproductive mass is limited to 5 % of shoot mass in total. The same resource conversion rate, g, is used for reproductive and vegetative biomass.

Eqs. (7.2.1) – (7.2.6) are applied to shoot and root ZOIs independently, with the difference that for root growth the factor fleaf is always one. We assume that the minimum uptake of above- and below-ground resources limits plant growth (Lehsten and Kleyer, 2007) and introduced adaptive shoot-root allocation in a way that more resources are allocated to the growth of the plant compartment that harvests the limiting resource (Weiner, 2004). For resource partitioning, we adopt the model of Johnson (1985) which assumes that the fraction of resources allocated to shoot growth is calculated as

$$\alpha_{shoot} = \frac{\Delta res_B}{\Delta res_B + \Delta res_A} \quad \text{Eq. (7.2.7)}$$

where Δres_A is above-ground and Δres_B is below-ground resource uptake.

Plants suffer resource stress if their resource uptake (in any layer) is below a fixed threshold fraction (thr_{res}) of their optimal uptake, which is calculated as maximum resource utilization times ZOI area. That means each week the condition

$\Delta res < thr_{res} * A_{shoot/root} * ru_{max}$

is evaluated and if it is true either for shoot or root the plant is considered as stress exposed during this week, and the state variable "duration of stress exposure", w_{stress}, is incremented. Consecutive weeks of resource stress linearly increase the probability of death

$$p_{mort} = p_{base} + \frac{w_{stress}}{surv_{max}} \quad \text{Eq. (7.2.8)}$$

where $surv_{max}$ is the maximum number of weeks a plant can survive under stress exposure and p_{base} is the stress independent background mortality of 0.7 % per week corresponding to an annual mortality rate of 20 % (Schippers et al., 2001). In order to increase the mean number of PFTs, we extended plant mortality by introducing density dependent background mortality. We multiplied p_{base} by a density dependent factor:

p_(base_new)=p_base*(1+e^((5*current abundance)/(maximal abundance))) Eq. (7.2.9)

Current abundance is the number of individuals of a PFT existing in the current time step; maximal abundance the potential number of full-grown individuals on the patch in monoculture. A factor of 5 was selected by pattern oriented modelling. Lower factors did not lead to the desired effect of slightly increasing the coexistence/mean number of frequent PFT; higher factors resulted in too strong effects on mortality. Without this extension, plant communities consisted only of 5-6 dominant PFTs. By expert judgement, one would expect a higher number of PFTs in such highly disturbed and nutrient rich environments. By adding that density dependent mortality, mean PFT number increased to 10 frequent PFTs.

Dead plants do not grow and reproduce anymore, but they still can shade others and are therefore still considered for above-ground competition. Each week the mass of all dead plants is reduced by 50 % and they are removed from the grid completely as soon as their total mass decreases below 10 mg.

Growth, dispersal and establishment of spacers of clonal plant types

For each individual (i.e. ramet) one spacer can grow at a time step. Analogously to generative reproduction, but in each week except for weeks of generative reproduction, 5% of resources acquired by the individual (Δres) are allocated to the growth of the spacer. First, the direction and distance of spacer growth is determined. The direction in which the spacer grows is chosen randomly from a uniform distribution. The distance of spacer growth is randomly chosen from a normal distribution, but the mean distance (SpacerL) is type-specific. The actual distance a spacer grows per week is calculated following:

$$\Delta SpacerL = \Delta res * 0.05 * g / mSpacer \qquad \text{Eq. (7.2.10)}$$

where g is a constant conversion rate between resource units and plant biomass (see above) and mSpacer is a type unspecific spacer mass of 70 mg per cm; this value was derived as mean of spacer masses of Phragmites australis (Granéli et al., 1992) and different sea grass species (Marbà et al., 2002). If the determined distance the spacer has to grow is reached and the respective cell is not the centre of another individual, spacer growth stops and the new ramet can establish with a fixed probability (p_{ram}) (see sub-model "Seed production, dispersal, and establishment" below). If the reached cell is occupied by the centre of a different plant, spacer growth continues randomly within a radius of two cells.

Resource sharing

Clonal plants of the integrator-type (sensu Oborny et al., 2000) share resources throughout the whole genet. Thereby each ramet provides above- and below-ground resources that are not essential for its own survival. The minimum resources (Res_{min}) a ramet needs for survival are calculated as a fixed threshold fraction (thr_{res}) of the ramet´s optimal uptake analogously to the threshold fraction which determines resource stress (see above Plant growth and mortality).

$$Res_{min} = thr_{res} * A_{shoot/root} * ru_{max}. \qquad \text{Eq. (7.2.11)}$$

Surplus resources are added for all ramets of the genet and hence equally shared among ramets. Ramets of non-integrator clonal plant types behave like non-clonal plant individuals in this respect, i.e. they do not share resources.

Seed production, dispersal and establishment

All plants disperse their seeds in week 20 each year. Seed number is determined by dividing reproductive mass by the average mass of one seed (Lehsten and Kleyer, 2007; Schippers et al., 2001). For each seed, dispersal distance is drawn from a log-normal, and direction from a uniform distribution (Stoyan and Wagner, 2001). Note that to avoid edge effects periodic boundary conditions are used.

Germination and seedling establishment are limited to four weeks in autumn directly after dispersal and four weeks in spring of the next year for all PFTs. In between, a winter mortality of 50 % of seeds is assumed and all seeds which did not germinate in these two seasons are removed.

Seedling recruitment is separated in two consecutive processes: (i) Seed germination and (ii) seedling competition. Germination is only allowed in grid cells that are not covered by any plant or its above-ground ZOI. In such cells, seeds germinate with a fixed probability (p_{germ}) and are converted to seedlings. In each cell only a single plant is allowed to establish. Seedling competition is modelled as a weighted lottery, using seed mass as a measure of competitive ability between seedlings (Chesson and Warner, 1981; Schippers et al., 2001). The seedling that is chosen for establishment is converted into a plant with a shoot and root mass equal to seed mass. All other seedlings, which germinated within the cell, die and are removed from the grid.

At the end of the vegetation period all growing spacers of clonal individuals establish with a fixed probability (p_{ram}) unless the cell they have reached by the time is occupied by the centre of a different individual already. If this is the case, the spacer is removed from the grid.

Disturbances

(1) grazing Grazing is modelled as partial removal of an individual's above-ground biomass. The frequency of grazing is specified by a constant weekly probability (p_{graz}) of a grazing event. Grazing is a process that acts selectively towards trait attributes such as shoot size and tissue properties. Therefore, for each plant the susceptibility to grazing (s_{graz}) is calculated as a function of shoot size, geometry and PFT-specific palatability (palat).

$$s_{graz} = m_{shoot} \cdot f_{leaf}^{-1} \cdot palat \quad \text{Eq. (7.2.12)}$$

The probability for each plant to be grazed within one a grazing event is derived by dividing individual susceptibilities by the current maximum individual susceptibility of all plants. All plants are checked for grazing in random order. In case a plant is grazed, 50 % of its shoot mass and its complete reproductive mass are removed. The random choice of plants is repeated for all other plants until 50 % of the total (aboveground) biomass on the whole grid has been removed. When all plants have been checked for grazing once, but less than 50% of the total above-ground biomass has been removed, grazing probabilities for all individuals are calculated once more based on Eq. (7.2.12) and the whole procedure is repeated until 50% of aboveground biomass has been removed or until a residual biomass is reached which is considered not grazable. This fraction is set to 15 g/m² following Schwinning and Parsons (1999). This allows a plant individual to be grazed never or several times during one week with a grazing event.

In addition to stochastic grazing, each year at the end of the vegetation period 50 % of the above-ground mass of all plant individuals is removed to mimic vegetation dieback in winter.

(2) TRAMPLING Trampling is integrated to account for effects of crossing vehicles, pedestrians or larger animals. Disturbances related to trampling are subdivided in small patches of 10x10 cm² that are randomly distributed on the overall grid. Each week a given percentage of the total area is prone to trampling and plant individuals from the disturbed patches are removed.

(3) CUTTING Depending on the management regime, cutting events are simulated one to three times during the vegetation period. During a week of simulated cutting, aboveground biomass of the patch is reduced to 500 mg/m². Cutting occurs either in autumn (1 cutting event per year), spring and autumn (2 cutting events per year) or in spring, summer and autumn (3 cutting events per year).

(4) HERBICIDE EFFECTS To include effects of herbicide exposure on plant individuals in IBC-grass, toxicological sub-processes are included. Several processes are potentially influenced by an herbicide effect: Mortality of plants, biomass of seedlings and plants, establishment of seedlings, seed production and seed fertility (i.e. sterility).

- **Plants suffer from an additional, herbicide-induced mortality probability. The strength of effect (p_{herb}) is determined by the specific effect intensity and is added after the density-dependent mortality.**
- **The biomass of seedlings and biomass gain of plants is reduced according to the specific effect intensity (growthFac).**
- **The establishment probability of seedlings is reduced by the specific effect intensity survFac.**
- **The resources available for seed production are reduced by the specific effect inten-**

sity (AllocSeedFac). The PFT specific seed weight is kept constant, resulting in a lower number of produced seeds.

- Seed sterility is increased by adding an herbicide-induced seed mortality probability according to the specific effect intensity (survFacSE), which is comparable to seed fertility.

The specific effect intensities of the different attributes are stored in an individual herbicide effect profile. To also include generation carry over effects (Boutin et al, 2014), produced seeds (F1 generation) inherit the effect profile of the mother plant (P generation).

Herbicide application is simulated in the first week of each simulated year, bearing in mind that only the growing season starting in spring is simulated in IBC-grass. In this week, the individual herbicide effect profile based on the scenario settings is assigned to the individual plants and seeds. However, each of the herbicide-induced effects appears only within the first week of the specific process (e.g. seed production is simulated only in week 25, therefore the herbicide effect on seed production occurs within this week).

In order to account for different species specific herbicide susceptibilities, we tested different affected PFT groups.

- All PFTs: All PFTs within the community are affected. This accounts for a broad spectrum herbicide. (N=55)
- Competitive PFTs: Only competitive PFTs, which occur frequently (in more than 80% of the control Monte Carlo runs) in an isolated community, are affected. This scenario was chosen to analyse the sensitivity of the community, and does not represent a realistic scenario. Selectiveness of herbicides is mostly based on other trait characteristics of plants, e.g. monocotyledonous vs dicotyledonous species. (N=4)
- Less-competitive PFTs: Only less-competitive PFTs, which occur frequently (in more than 80% of the control Monte Carlo runs) in an isolated community, are affected. This scenario is used to analyse the sensitivity of the community as a comparison to the ‘competitive PFTs’ scenario and probably does not represent a realistic case. (N=4)
- Monocotyledonous PFTs: Only monocotyledonous PFTs are affected. This scenario accounts for a selective herbicide acting only on monocotyledonous PFTs. (N=14)
- Dicotyledonous PFTs: Only dicotyledonous PFTs are affected. This scenario accounts for a selective herbicide acting only on dicotyledonous PFTs. (N=40)

The PFTs within these groups have the same herbicide susceptibility (=1). Therefore the effect intensity is equal for each individual of the affected PFT. The distinction between monocotyledonous and dicotyledonous PFTs involves only the herbicide susceptibility (0/1) but no other trait characteristics.

REFERENCES

Berendse, F., 1983. Interspecific Competition and Niche Differentiation Between Plantago Lanceolata and Anthoxanthum Odoratum in a Natural Hayfield. J. Ecol. 71, 379. doi:10.2307/2259721

Chesson, P., 2000. Mechanisms of maintenance of species diversity. Annu. Rev. Ecol. Syst. 31, 343–366. doi:10.1146/annurev.ecolsys.31.1.343

Chesson, P.L., Warner, R.R., 1981. Environmental Variability Promotes Coexistence in Lottery Competitive Systems. Am. Nat. 117, 923. doi:10.1086/283778

Granéli, W., Weisner, S.B., Sytsma, M., 1992. Rhizome dynamics and resource storage in Phragmites australis. Wetl. Ecol. Manag. 1. doi:10.1007/BF00244929

Grimm, V., Berger, U., Bastiansen, F., Eliassen, S., Ginot, V., Giske, J., Goss-Custard, J., Grand, T., Heinz, S.K., Huse, G., Huth, A., Jepsen, J.U., Jørgensen, C., Mooij, W.M., Müller, B., Pe'er, G., Piou, C., Railsback, S.F., Robbins, A.M., Robbins, M.M., Rossmanith, E., Rüger, N., Strand, E., Souissi, S., Stillman, R.A., Vabø, R., Visser, U., DeAngelis, D.L., 2006. A standard protocol for describing individual-based and agent-based models. Ecol. Modell. 198, 115–126. doi:10.1016/j.ecolmodel.2006.04.023

Grimm, V., Berger, U., DeAngelis, D.L., Polhill, J.G., Giske, J., Railsback, S.F., 2010. The ODD protocol: A review and first update. Ecol. Modell. 221, 2760–2768. doi:10.1016/j.ecolmodel.2010.08.019

Johnson, I.R., 1985. A Model of the Partitioning of Growth between the Shoots and Roots of Vegetative Plants. Ann. Bot. 55, 421–431.

Körner, K., Pfestorf, H., May, F., Jeltsch, F., 2014. Modelling the effect of belowground herbivory on grassland diversity. Ecol. Modell. 273, 79–85. doi:10.1016/j.ecolmodel.2013.10.025

Lehsten, V., Kleyer, M., 2007. Turnover of plant trait hierarchies in simulated community assembly in response to fertility and disturbance. Ecol. Modell. 203, 270–278. doi:10.1016/j.ecolmodel.2006.11.034

Marbà, N., Hemminga, M., Mateo, M., Duarte, M., Mass, Y., Terrados, J., Gacia, E., 2002.

Carbon and nitrogen translocation between seagrass ramets. Mar. Ecol. Prog. Ser. 226, 287–300. doi:10.3354/meps226287

May, F., Grimm, V., Jeltsch, F., 2009. Reversed effects of grazing on plant diversity: the role of below-ground competition and size symmetry. Oikos 118, 1830–1843. doi:10.1111/j.1600-0706.2009.17724.x

Oborny, B., Kun, a., Czárá, T., Bokros, S., 2000. The effect of clonal integration on plant competition for mosaic habitat space. Ecology 81, 3291–3304. doi:10.1890/0012-9658(2000)081[3291:TEOCIO]2.0.CO;2

OECD, 2006a. Test No. 227: Terrestrial Plant Test: Vegetative Vigour Test, in: OECD Guidelines for the Testing of Chemicals, Section 2. OECD Publishing, Paris.

OECD, 2006b. Test No. 208: Terrestrial Plant Test: Seedling Emergence and Seedling Growth Test, in: OECD Guidelines for the Testing of Chemicals, Section 2. OECD Publishing, Paris.

Reeg, J., Schad, T., Preuss, T.G., Solga, A., Körner, K., Mihan, C., Jeltsch, F., 2017. Modelling direct and indirect effects of herbicides on non-target grassland communities. Ecol. Modell. 348, 44–55. doi:10.1016/j.ecolmodel.2017.01.010

Schad, T., 2013. Xplicit – A Modelling Framework for Ecological Risk Characterisation at Landscape-scales in Regulatory Risk Assessment and Risk Management of Plant Protection Products.

Schad, T., Schulz, R., 2011. Xplicit, a novel approach in probabilistic spatiotemporally explicit exposure and risk assessment for plant protection products. Integr. Environ. Assess. Manag. 7, 612–23. doi:10.1002/ieam.205

Schippers, P., van Groenendael, J.M., Vleeshouwers, L.M., Hunt, R., 2001. Herbaceous plant strategies in disturbed habitats. Oikos 95, 198–210. doi:10.1034/j.1600-0706.2001.950202.x

Schwinning, S., Parsons, A.J., 1999. The stability of grazing systems revisited: spatial models and the role of heterogeneity. Funct. Ecol. 13, 737–747. doi:10.1046/j.1365-2435.1999.00382.x

Silvertown, J., 2004. Plant coexistence and the niche. Trends Ecol. Evol.

Stoyan, D., Wagner, S., 2001. Estimating the fruit dispersion of anemochorous forest trees. Ecol. Modell. 145, 35–47. doi:10.1016/S0304-3800(01)00385-4

Weiner, J., 2004. Allocation, plasticity and allometry in plants. Perspect. Plant Ecol. Evol.

Syst. 6, 207–215. doi:10.1078/1433-8319-00083

Weiner, J., Stoll, P., Muller-Landau, H., Jasentuliyana, A., 2001. The effects of density, spatial pattern, and competitive symmetry on size variation in simulated plant populations. Am. Nat. 158, 438–50. doi:10.1086/321988

Weiß, L., Pfestorf, H., May, F., Körner, K., Boch, S., Fischer, M., Müller, J., Prati, D., Socher, S.A., Jeltsch, F., 2014. Grazing response patterns indicate isolation of semi-natural European grasslands. Oikos 123, 599–612. doi:10.1111/j.1600-0706.2013.00957.x

7.2.2 PFT classification

Table 7.7: Classification of plant species into plant functional types (PFT) according to trait characteristics (see Table 3.1). Dicotyledonous (di) and monocotyledonous (mo) only differ in their herbicide susceptibility in some simulation scenarios.

Species	Maximum plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	Cotyledons	PFT ID
Heracleum sphondylium	large	semi-rosette	competitor	intermediate	aclonal	-	-	di	PFT LSCId
Arrhenatherum elatius	large	semi-rosette	competitor	intermediate	clonal	short	yes	mo	PFT LSCIcl1m
Anthriscus sylvestris	large	semi-rosette	competitor	intermediate	clonal	short	no	di	PFT LSCIcl2d
Filipendula ulmaria	large	semi-rosette	competitor	intermediate	clonal	long	yes	di	PFT LSCIcl3d
Daucus carota	medium	semi-rosette	competitor	intermediate	aclonal	-	-	di	PFT MSCId
Leucanthemum vulgare	medium	semi-rosette	competitor	intermediate	clonal	long	yes	di	PFT MSCIcl3d
Silene vulgaris	small	semi-rosette	competitor	intermediate	clonal	short	yes	di	PFT SSCIcl1d
Phalaris arundinacea	large	erect	competitor	intermediate	clonal	long	yes	mo	PFT LECIcl3m
Vicia cracca	large	erect	competitor	intermediate	clonal	long	yes	di	PFT LECIcl3d
Lathyrus pratensis	medium	erect	competitor	intermediate	clonal	long	yes	di	PFT MECIcl3d
Vicia sepium	medium	erect	competitor	intermediate	clonal	long	yes	di	PFT MECIcl3d
Galium mollugo agg.	medium	erect	competitor	intermediate	clonal	long	no	di	PFT MECIcl4d
Cirsium vulgare	large	semi-rosette	competitor	avoider	aclonal	-	-	di	PFT LSCAd
Rumex crispus	medium	semi-rosette	competitor	avoider	aclonal	-	-	di	PFT MSCAd
Deschampsia cespitosa	medium	semi-rosette	competitor	avoider	clonal	short	yes	mo	PFT MSCAcl1m
Rumex obtusifolius	medium	semi-rosette	competitor	avoider	clonal	short	yes	di	PFT MSCAcl1d
Senecio jacobaea	medium	semi-rosette	competitor	avoider	clonal	short	yes	di	PFT MSCAcl1d
Lolium perenne	medium	semi-rosette	competitor	avoider	clonal	short	no	mo	PFT MSCAcl2m
Achillea millefolium	medium	semi-rosette	competitor	avoider	clonal	long	yes	di	PFT MSCAcl3d
Agrostis gigantea	medium	semi-rosette	competitor	avoider	clonal	long	yes	mo	PFT MSCAcl3m
Festuca rubra	medium	semi-rosette	competitor	avoider	clonal	long	yes	mo	PFT MSCAcl3m
Poa pratensis	medium	semi-rosette	competitor	avoider	clonal	long	yes	mo	PFT MSCAcl3m
Urtica dioica	large	erect	competitor	avoider	clonal	long	no	di	PFT LECAcl4d
Cirsium arvense	medium	erect	competitor	avoider	clonal	long	no	di	PFT MECAcl4d

Species	Maximum plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	Cotyledons	PFT ID
Equisetum arvense	small	erect	competitor	avoider	clonal	long	yes	fa	PFT SECAcl3
Plantago lanceolata	medium	rosette	intermediate	tolerator	clonal	short	yes	di	PFT MRITcl1d
Potentilla reptans	small	rosette	intermediate	tolerator	clonal	long	yes	di	PFT SRITcl3d
Tussilago farfara	small	rosette	intermediate	tolerator	clonal	long	yes	di	PFT SRITcl3d
Agrostis capillaris	medium	semi-rosette	intermediate	tolerator	clonal	long	yes	mo	PFT MSITcl3m
Poa trivialis	medium	semi-rosette	intermediate	tolerator	clonal	long	no	mo	PFT MSITcl4m
Lotus corniculatus	medium	erect	intermediate	tolerator	aclonal	-	-	di	PFT MEITd
Cerastium fontanum	small	erect	intermediate	tolerator	clonal	short	yes	di	PFT SEITcl1d
Veronica chamaedrys	small	erect	intermediate	tolerator	clonal	long	yes	di	PFT SEITcl3d
Glechoma hederacea	small	erect	intermediate	tolerator	clonal	long	no	di	PFT SEITcl4d
Artemisia vulgaris	large	semi-rosette	competitor	tolerator	aclonal	-	-	di	PFT LSCTd
Tragopogon pratensis	medium	semi-rosette	intermediate	intermediate	aclonal	-	-	di	PFT MSIId
Salvia pratensis	medium	semi-rosette	intermediate	intermediate	clonal	short	yes	di	PFT MSIIcl1d
Myosotis arvensis	small	semi-rosette	intermediate	intermediate	aclonal	-	-	di	PFT SSIId
Leontodon autumnalis	small	rosette	intermediate	avoider	clonal	short	yes	di	PFT SRIAcl1d
Plantago major	small	rosette	intermediate	avoider	clonal	short	yes	di	PFT SRIAcl1d
Taraxacum sect. Ruderalia	small	rosette	intermediate	avoider	clonal	short	yes	di	PFT SRIAcl1d
Potentilla anserina	small	rosette	intermediate	avoider	clonal	long	yes	di	PFT SRIAcl3d
Bellis perennis	small	rosette	intermediate	avoider	clonal	long	no	di	PFT SRIAcl4d
Elymus repens	large	semi-rosette	competitor	tolerator	clonal	long	yes	mo	PFT LSCTcl3m
Festuca arundinacea	large	semi-rosette	competitor	tolerator	clonal	long	yes	mo	PFT LSCTcl3m
Holcus mollis	medium	semi-rosette	intermediate	avoider	clonal	long	yes	mo	PFT MSIAcl3m
Agrostis stolonifera	medium	semi-rosette	intermediate	avoider	clonal	long	no	mo	PFT MSIAcl4m
Ranunculus repens	medium	semi-rosette	intermediate	avoider	clonal	long	no	di	PFT MSIAcl4d
Trifolium repens	small	semi-rosette	intermediate	avoider	clonal	long	no	di	PFT SSIAcl4d
Polygonum aviculare	small	erect	intermediate	avoider	aclonal	-	-	di	PFT SEIAd
Lamium album	small	erect	intermediate	avoider	clonal	long	no	di	PFTSEIAcl4d
Festuca pratensis	medium	semi-rosette	competitor	tolerator	clonal	short	yes	mo	PFT MSCTcl1m

Species	Maximum plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	Cotyledons	PFT ID
Holcus lanatus	medium	semi-rosette	competitor	tolerator	clonal	short	yes	mo	PFT MSCTcl1m
Phleum pratense	medium	semi-rosette	competitor	tolerator	clonal	short	yes	mo	PFT MSCTcl1m
Ranunculus acris	medium	semi-rosette	competitor	tolerator	clonal	short	yes	di	PFT MSCTcl1d
Centaurea jacea	medium	semi-rosette	competitor	tolerator	clonal	short	no	di	PFT MSCTcl2d
Dactylis glomerata	medium	semi-rosette	competitor	tolerator	clonal	short	no	mo	PFT MSCTcl2m
Rumex acetosa	medium	semi-rosette	competitor	tolerator	clonal	short	no	di	PFT MSCTcl2d
Trifolium pratense	small	semi-rosette	competitor	tolerator	aclonal	-	-	di	PFT SSCTd
Galium verum	medium	erect	stress-tolerator	tolerator	clonal	long	yes	di	PFT MESTcl3d
Stellaria graminea	small	erect	stress-tolerator	tolerator	clonal	long	no	di	PFT SESTcl4d
Poa angustifolia	medium	semi-rosette	stress-tolerator	avoider	clonal	long	no	mo	PFT MSSAcl4m
Hypericum perforatum	medium	erect	competitor	tolerator	aclonal	-	-	di	PFT MECTd
Alopecurus pratensis	medium	erect	competitor	tolerator	clonal	long	yes	mo	PFT MECTcl3m
Cerastium holosteoides	small	erect	competitor	tolerator	aclonal	-	-	di	PFT SECTd
Cerastium arvense	small	erect	competitor	tolerator	clonal	long	yes	di	PFT SECTcl3d

7.3 Supplemental material of chapter 4

7.3.1 Species lists

Table 7.8: **Species list of field boundary community.** Based on a literature review by Kolja Bergolz (unpublished). Only perennial species, which occurred in >25% of the studies were selected.

Species	Maximal plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	PFT ID
Heracleum sphondylium	large	semi-rosette	competitor	intermediate	aclonal	-	-	PFT13
Arrhenatherum elatius	large	semi-rosette	competitor	intermediate	clonal	short	yes	PFT13clonal1
Anthriscus sylvestris	large	semi-rosette	competitor	intermediate	clonal	short	no	PFT13clonal2
Filipendula ulmaria	large	semi-rosette	competitor	intermediate	clonal	long	yes	PFT13clonal3
Daucus carota	medium	semi-rosette	competitor	intermediate	aclonal	-	-	PFT14
Leucanthemum vulgare	medium	semi-rosette	competitor	intermediate	clonal	long	yes	PFT14clonal3
Silene vulgaris	small	semi-rosette	competitor	intermediate	clonal	short	yes	PFT15clonal1
Phalaris arundinacea, Vicia cracca	large	erect	competitor	intermediate	clonal	long	yes	PFT16clonal3
Lathyrus pratensis, Vicia sepium	medium	erect	competitor	intermediate	clonal	long	yes	PFT17clonal3
Galium mollugo agg.	medium	erect	competitor	intermediate	clonal	long	no	PFT17clonal4
Cirsium vulgare	large	semi-rosette	competitor	avoider	aclonal	-	-	PFT22
Rumex crispus	medium	semi-rosette	competitor	avoider	aclonal	-	-	PFT23
Deschampsia cespitosa, Rumex obtusifolius, Senecio jacobaea	medium	semi-rosette	competitor	avoider	clonal	short	yes	PFT23clonal1
Lolium perenne	medium	semi-rosette	competitor	avoider	clonal	short	no	PFT23clonal2
Achillea millefolium, Agrostis gigantea, Festuca rubra, Poa pratensis	medium	semi-rosette	competitor	avoider	clonal	long	yes	PFT23clonal3
Urtica dioica	large	erect	competitor	avoider	clonal	long	no	PFT25clonal4
Cirsium arvense	medium	erect	competitor	avoider	clonal	long	no	PFT26clonal4
Equisetum arvense	small	erect	competitor	avoider	clonal	long	yes	PFT27clonal3
Plantago lanceolata	medium	rosette	intermediate	tolerator	clonal	short	yes	PFT29clonal1
Potentilla reptans, Tussilago farfara	small	rosette	intermediate	tolerator	clonal	long	yes	PFT30clonal3

Species	Maximal plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	PFT ID
Agrostis capillaris	medium	semi-rosette	intermediate	tolerator	clonal	long	yes	PFT32clonal3
Poa trivialis	medium	semi-rosette	intermediate	tolerator	clonal	long	no	PFT32clonal4
Lotus corniculatus	medium	erect	intermediate	tolerator	aclonal	-	-	PFT35
Cerastium fontanum	small	erect	intermediate	tolerator	clonal	short	yes	PFT36clonal1
Veronica chamaedrys	small	erect	intermediate	tolerator	clonal	long	yes	PFT36clonal3
Glechoma hederacea	small	erect	intermediate	tolerator	clonal	long	no	PFT36clonal4
Artemisia vulgaris	large	semi-rosette	competitor	tolerator	aclonal	-	-	PFT4
Tragopogon pratensis	medium	semi-rosette	intermediate	intermediate	aclonal	-	-	PFT41
Salvia pratensis	medium	semi-rosette	intermediate	intermediate	clonal	short	yes	PFT41clonal1
Myosotis arvensis	small	semi-rosette	intermediate	intermediate	aclonal	-	-	PFT42
Leontodon autumnalis, *Plantago major,* *Taraxacum sect. Ruderalia*	small	rosette	intermediate	avoider	clonal	short	yes	PFT48clonal1
Potentilla anserina	small	rosette	intermediate	avoider	clonal	long	yes	PFT48clonal3
Bellis perennis	small	rosette	intermediate	avoider				PFT48clonal4
Elymus repens, Festuca arundinacea	large	semi-rosette	competitor	tolerator	clonal	long	yes	PFT4clonal3
Holcus mollis	medium	semi-rosette	intermediate	avoider	clonal	long	yes	PFT50clonal3
Agrostis stolonifera, Ranunculus repens	medium	semi-rosette	intermediate	avoider	clonal	long	no	PFT50clonal4
Trifolium repens	small	semi-rosette	intermediate	avoider	clonal	long	no	PFT51clonal4
Polygonum aviculare	small	erect	intermediate	avoider				PFT54
Lamium album	small	erect	intermediate	avoider	clonal	long	no	PFT54clonal4
Festuca pratensis, Holcus lanatus, Phleum pratense, Ranunculus acris	medium	semi-rosette	competitor	tolerator	clonal	short	yes	PFT5clonal1
Centaurea jacea, Dactylis glomerata, Rumex acetosa	medium	semi-rosette	competitor	tolerator	clonal	short	no	PFT5clonal2

Species	Maximal plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	PFT ID
Trifolium pratense	small	semi-rosette	competitor	tolerator	aclonal	-	-	PFT6
Galium verum	medium	erect	stress-tolerator	tolerator	clonal	long	yes	PFT62clonal3
Stellaria graminea	small	erect	stress-tolerator	tolerator	clonal	long	no	PFT63clonal4
Poa angustifolia	medium	semi-rosette	stress-tolerator	avoider	clonal	long	no	PFT77clonal4
Hypericum perforatum	medium	erect	competitor	tolerator	aclonal	-	-	PFT8
Alopecurus pratensis	medium	erect	competitor	tolerator	clonal	long	yes	PFT8clonal3
Cerastium holosteoides	small	erect	competitor	tolerator	aclonal	-	-	PFT9
Cerastium arvense	small	erect	competitor	tolerator	clonal	long	yes	PFT9clonal3

Table 7.9: Species list of the *Arrhenatheretalia* community

Species	Maximum plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	PFT ID
Heracleum sphondylium,	large	semi-rosette	competitor	intermediate	aclonal	-	-	PFT13
Daucus carota								
Angelica sylvestris, Arrhenatherum elatius	large	semi-rosette	competitor	intermediate	clonal	short	yes	PFT13clonal1
Anthriscus sylvestris	large	semi-rosette	competitor	intermediate	clonal	short	no	PFT13clonal2
Crepis biennis, Knautia arvensis	medium	semi-rosette	competitor	intermediate	aclonal	-	-	PFT14
Geranium pratense, Pimpinella major	medium	semi-rosette	competitor	intermediate	clonal	short	yes	PFT14clonal1
Leucanthemum vulgare s.l.								PFT14clonal3
Vicia cracca	large	erect	competitor	intermediate	clonal	long	yes	PFT16clonal3
Lathyrus pratensis, Vicia sepium	medium	erect	competitor	intermediate	clonal	long	yes	PFT17clonal3
Galium mollugo s.l.	medium	erect	competitor	intermediate	clonal	long	no	PFT17clonal4
Cirsium paulstre	large	semi-rosette	competitor	avoider	aclonal	-	-	PFT22
Achillea millefolium, Poa pratensis, Festuca rubra	medium	semi-rosette	competitor	avoider	clonal	long	yes	PFT23clonal3

Species	Maximum plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	PFT ID
Plantago lanceolata	medium	rosette	intermediate	tolerator	clonal	short	yes	PFT29clonal1
Leontodon hispidus	small	erect	intermediate	tolerator	clonal	short	yes	PFT30clonal1
Anthoxanthum odoratum	medium	semi-rosette	intermediate	tolerator	clonal	short	yes	PFT32clonal1
Agrostis capillaris, Trisetum flavescens	medium	semi-rosette	intermediate	tolerator	clonal	long	yes	PFT32clonal3
Poa trivialis	medium	semi-rosette	intermediate	tolerator	clonal	long	no	PFT32clonal4
Ranunculus bulbosus	small	semi-rosette	intermediate	tolerator	clonal	short	no	PFT33clonal2
Briza media, Luzula campestris	small	semi-rosette	intermediate	tolerator	clonal	long	yes	PFT33clonal3
Ajuga reptans	small	semi-rosette	intermediate	tolerator	clonal	long	no	PFT33clonal4
Lotus corniculatus, Lotus pedunculatus	medium	erect	intermediate	tolerator	aclonal	-	-	PFT35
Veronica chamaedrys	small	erect	intermediate	tolerator	clonal	long	yes	PFT36clonal3
Veronica arvensis	small	erect	intermediate	tolerator	clonal	long	no	PFT36clonal4
Carum carvi	large	semi-rosette	competitor	tolerator	aclonal	-	-	PFT4
Tragopogon pratensis, Campanula patula	medium	semi-rosette	intermediate	intermediate	aclonal	-	-	PFT41
Taraxacum officinale agg.	small	rosette	intermediate	avoider	aclonal	-	-	PFT48
Plantago media	small	rosette	intermediate	avoider	clonal	short	yes	PFT48clonal1
Colchicum autumnale, Hypochaeris radicata	small	rosette	intermediate	avoider	clonal	short	no	PFT48clonal2
Bellis perennis	small	rosette	intermediate	avoider	clonal	long	no	PFT48clonal4
Cynosorus cristatus	medium	semi-rosette	intermediate	avoider	clonal	short	yes	PFT50clonal1
Cardamine pratensis, Trifolium repens	small	semi-rosette	intermediate	avoider	clonal	long	no	PFT51clonal4
Prunella vulgaris	small	erect	intermediate	avoider	clonal	long	no	PFT54clonal4
Bistorta officinalis	medium	semi-rosette	stress-tolerator	tolerator	clonal	long	yes	PFT59clonal3

Species	Maximum plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	PFT ID
Festuca pratensis, Holcus lanatus, Ranunculus acris, Trollius europaeus	medium	semi-rosette	competitor	tolerator	clonal	short	yes	PFT5clonal1
Centaurea jacea, Dactylis glomerata, Rumex acetosa	medium	semi-rosette	competitor	tolerator	clonal	short	no	PFT5clonal2
Helictotrichon pubescens	medium	semi-rosette	competitor	tolerator	clonal	long	yes	PFT5clonal3
Trifolium pratense	small	semi-rosette	competitor	tolerator	aclonal	-	-	PFT6
Achillea ptarmica	medium	erect	stress-tolerator	tolerator	clonal	long	yes	PFT62clonal1
Sanguisorba officinalis	medium	semi-rosette	stress-tolerator	intermediate	clonal	short	yes	PFT68clonal1
Alopecurus pratensis	medium	erect	competitor	tolerator	clonal	long	yes	PFT8clonal3
Cerastium holosteoides	small	erect	competitor	tolerator	aclonal	-	-	PFT9

Table 7.10: Species list of the *Calthion* community

Species	Maximum plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	PFT ID
Cirsium oleraceum, Angelica sylvestris	large	semi-rosette	competitor	intermediate	clonal	long	yes	PFT13clonal1
Filipendula ulmaria	large	semi-rosette	competitor	intermediate	clonal	long	yes	PFT13clonal3
Crepis paludosa	medium	semi-rosette	competitor	intermediate	clonal	short	yes	PFT14clonal1
Vicia cracca	large	erect	competitor	intermediate	clonal	long	yes	PFT16clonal3
Lathyrus pratensis	medium	erect	competitor	intermediate	clonal	long	yes	PFT17clonal3
Juncus effusus	large	erect	competitor	avoider	clonal	long	yes	PFT19clonal3
Cirsium palustre	large	semi-rosette	competitor	avoider	aclonal			PFT22
Deschampsia cespitosa	large	semi-rosette	competitor	avoider	clonal	short	yes	PFT22clonal1
Achillea millefolium, Poa pratensis	medium	semi-rosette	competitor	avoider	clonal	long	yes	PFT23clonal3
Anthoxanthum odoratum	medium	semi-rosette	intermediate	tolerator	clonal	short	yes	PFT32clonal1
Carex panicea	medium	semi-rosette	intermediate	tolerator	clonal	long	yes	PFT32clonal3

Species	Maximum plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	PFT ID
Poa trivialis	medium	semi-rosette	intermediate	tolerator	clonal	long	no	PFT32clonal4
Myosotis nemorosa	small	semi-rosette	intermediate	tolerator	clonal	long	yes	PFT33clonal3
Ajuga reptans	small	semi-rosette	intermediate	tolerator	clonal	long	no	PFT33clonal4
Lotus pedunculatus	medium	erect	intermediate	tolerator	aclonal			PFT35
Galium uliginosum	small	erect	intermediate	tolerator	clonal	short	yes	PFT36clonal4
Epilobium palustre	medium	erect	intermediate	intermediate	clonal	long	no	PFT38clonal4
Agrostis canina, Silene flos-cuculi	medium	semi-rosette	intermediate	intermediate	clonal	long	yes	PFT41clonal3
Taraxacum officinale agg.	small	rosette	intermediate	avoider	aclonal	-	-	PFT48
Cerastium holosteoides	small	rosette	intermediate	avoider	clonal	short	no	PFT48clonal2
Bellis perennis	small	rosette	intermediate	avoider	clonal	long	no	PFT48clonal4
Bromus racemosus	large	semi-rosette	competitor	tolerator	clonal	short	no	PFT4clonal2
Caltha palustris	medium	semi-rosette	intermediate	avoider	clonal	short	yes	PFT50clonal1
Ranunculus flammula, Ranunculus repens	medium	semi-rosette	intermediate	avoider	clonal	long	no	PFT50clonal4
Colchicum autumnale, Trifolium repens	small	semi-rosette	intermediate	avoider	clonal	long	no	PFT51clonal4
Prunella vulgaris	small	erect	intermediate	avoider	clonal	long	no	PFT54clonal4
Cirsium rivulare, Juncus acutiflorus	large	semi-rosette	stress-tolerator	tolerator	clonal	long	yes	PFT58clonal3
Bistorta officinalis, Carex nigra	medium	semi-rosette	stress-tolerator	tolerator	clonal	long	yes	PFT59clonal3
Festuca pratensis, Holcus lanatus, Ranunculus acris, Trollius europaeus	medium	semi-rosette	competitor	tolerator	clonal	short	yes	PFT5clonal1
Cardamine pratensis, Rumex acetosa	medium	semi-rosette	competitor	tolerator	clonal	short	no	PFT5clonal2
Trifolium pratense	small	semi-rosette	competitor	tolerator	aclonal	-	-	PFT6
Achillea ptarmica	medium	erect	stress-tolerator	tolerator	clonal	long	yes	PFT62clonal1

Species	Maximum plant mass	Growth form	Resource response	Grazing response	Clonality	Lateral spread	Integration	PFT ID
Galium palustre	small	erect	stress-tolerator	intermediate	clonal	long	no	PFT66clonal4
Scirpus sylvaticus	large	semi-rosette	stress-tolerator	intermediate	clonal	long	yes	PFT67clonal3
Sanguisorba officinalis	medium	semi-rosette	stress-tolerator	intermediate	clonal	short	yes	PFT68clonal1
Alopecurus pratensis	medium	erect	competitor	tolerator	clonal	long	yes	PFT8clonal3
Centaurea jacea	small	erect	competitor	tolerator	aclonal	-	-	PFT9

7.3.2 ODD protocol

The model description follows the ODD (Overview, Design concepts, Details) protocol for describing individual- and agent-based models (Grimm et al., 2010, 2006). We based our simulation experiments on the grassland community model IBC-grass (May et al., 2009; Weiß et al., 2014), refined the latest version and extended it by introducing toxicological processes. Refined processes and extensions are marked in bold.

Purpose

This extended version of IBC-grass is designed to predict effects of herbicide exposure on a local perennial plant community adjacent to arable fields (field boundary).

Entities, state variables and scales

The model simulates plant community processes within an approx. 3 m² patch designed as a grid of 173*173 grid cells, i.e. one grid cell represents 1cm². Each grid cell can comprise several seeds and not more than one individual plant. Each seed is described with the state variable of its specific location on the grid and moreover its age and mass. An individual plant can either be a ramet of a clonal plant type or a non-clonal plant. Each plant individual is described by its specific position on the grid, the duration of resource stress exposure, the shoot, root and reproductive mass and the presence of growing spacers in case of clonal plant types. Plant individuals are categorized into plant functional types (PFT), which differ in their characteristics of 12 selected trait parameters. Plant individuals have circular area around their stem, the 'zone-of-influence' (ZOI). Within this area, plants acquire and compete for resources in the case of overlapping ZOIs. Two compartments (layers) are distinguished: above- and belowground. ZOIs are determined by the specific above- and belowground biomasses of the individual plant. As plants grow, the ZOI areas increase over time. One simulated time step represents one week; in each year 30 weeks of vegetation period are simulated.

Process overview and scheduling

The schedule of the simulated processes is shown in Figure 7.18. All processes except for seed dispersal, seedling establishment and cutting are executed each week. Seed dispersal, seedling establishment and cutting are limited to certain weeks within the year. Winter dieback of aboveground biomass and seed mortality is considered once at the end of each year. The plant's functional traits determine all processes. The state variable mass and age are synchronously updated each week and year after all model entities have been processed.

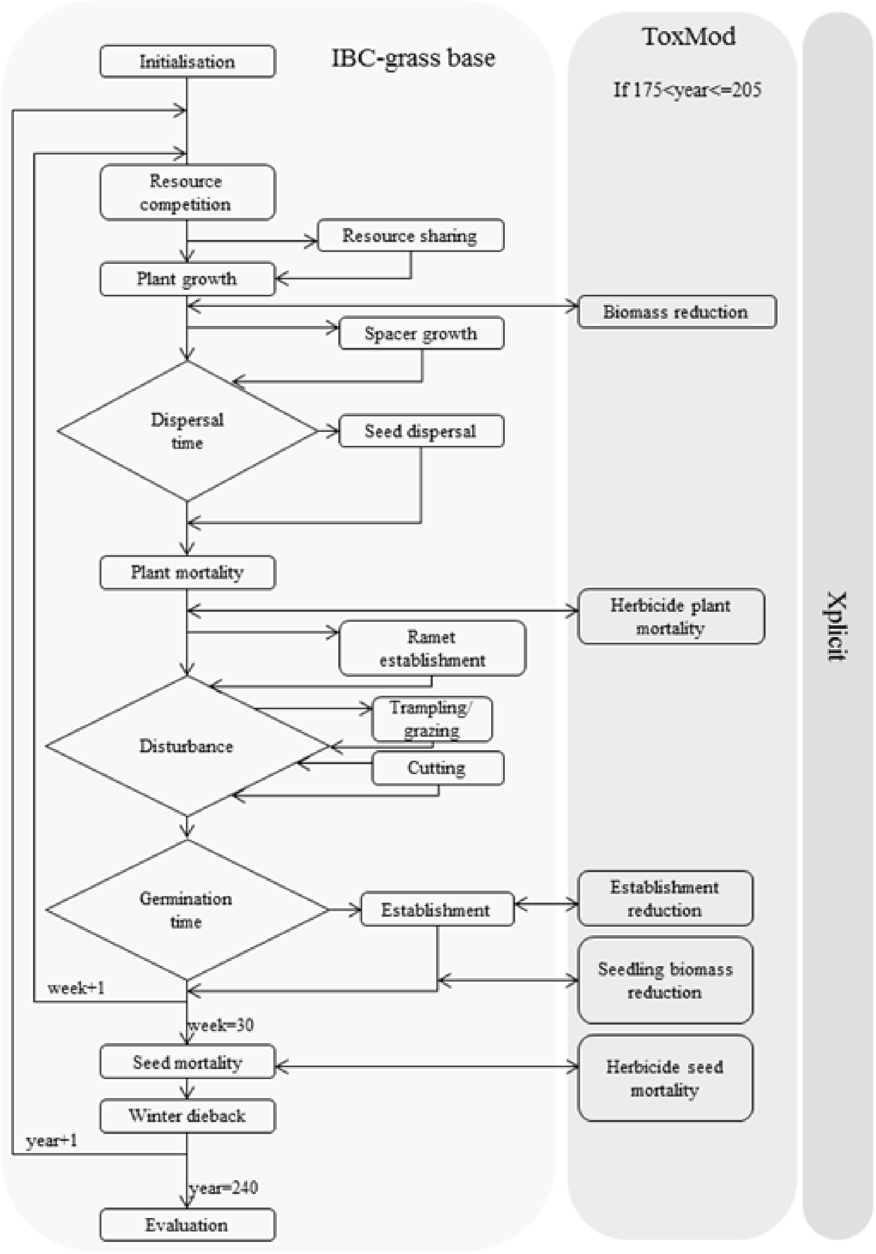

Figure 7.18: Flow chart of the processes within IBC-grass.

DESIGN CONCEPTS

BASIC PRINCIPLES

The model simulates local competition by using the zone-of-influence approach in two layers: aboveground and belowground. Thereby, it distinguishes between symmetric (belowground) and asymmetric (aboveground) competition. Competition among individuals of the same functional type (i.e. intra-PFT competition) is assumed to be higher than competition between individuals of different PFTs (i.e. inter-PFT competition) (Berendse, 1983). In this model version, density-dependent mortality is introduced.

EMERGENCE

Endpoints on community level, e.g. PFT diversity and biomass, emerge from individual plant-plant interactions, resource levels, disturbance events like trampling, grazing and cutting and herbicide exposure effects.

ADAPTATION

Plants balance the uptake of above- and belowground resources by adapting the allocation of resources to shoot and root growth.

INTERACTIONS

Plants compete for resources and space by the ZOI approach.

STOCHASTICITY

Demographic noise is included by modelling seed dispersal, seedling establishment, seed mortality and plant mortality stochastically. In addition, grazing and trampling occur randomly on the simulated grid. The plant's individual probability to be grazed is determined by its specific plant traits.

INITIALIZATION

Initially, ten seeds per PFT of the regional PFT pool (see Appendix A, Tables A.1-A.3) were randomly distributed over the grid. Their germination probability was set to 100% in order to have equal initial population sizes of all PFTs. Above- as well as belowground resources are distributed spatially and temporally homogenous.

INPUT

The model needs the information about the available PFT pool used in a simulation that includes external seed input and the trait characteristics of the respective PFTs. In addition, herbicide effects are introduced via an http-interface, which hands over species effect distributions generated by the model Xplicit (see sub-model "herbicide exposure effects").

SUB-MODELS

Most sub-models are adopted from the model version described by Weiß et al. (2014). New and modified sub-models are marked in bold.

COMPETITION.

Following the ZOI approach, plants compete for resources in a circular area around their central location point. To relate plant mass to the area covered (Ashoot), the allometric relation by Weiner et al. (2001) is used.

$$A_{shoot} = c_{shoot} \cdot \left(f_{leaf} \cdot m_{shoot}\right)^{2/3} \qquad \text{Eq. (7.3.1)}$$

Where cshoot is a constant ratio between leaf mass and ZOI area and mshoot is vegetative shoot mass. The factor fleaf is introduced to describe different shoot geometries and is defined as the ratio between photosynthetic active (leaf) and inactive (stem) tissue. Only the former is considered for the calculation of the ZOI size. These circular areas are projected onto a grid of discrete cells. Grid cells thus contain the information by which plants they are covered, so that resource competition can be calculated cell by cell. The resources within a cell are shared among plants according to their relative competition coefficients (β_i). The resource uptake (Δres) of plant i from a cell with resource availability (Res_{cell}) covered by n plants is thus calculated as

$$\Delta res_i = \frac{\beta_i}{\sum_{j=1}^{n} \beta_j} \cdot Res_{cell} \qquad \text{Eq. (7.3.2)}$$

Calculating β_i in different ways allows including different modes of competition, i.e. symmetric or asymmetric (Weiner et al., 2001). We assume that the relative competitive ability of a plant is correlated with its maximum growth rate in the absence of resource competition. Therefore β_i is proportional to maximum resource utilization per unit area covered (ru_{max}, see Sub-model "Plant growth and mortality"). In the case of size-symmetric competition, β_i simply equals rumax:

$$\beta_i = ru_{max} \qquad \text{Eq. (7.3.3)}$$

In the case of partially size-asymmetric competition β_i is a function of plant mass and shoot geometry:

$$\beta_i = ru_{max} \cdot m_{shoot} \cdot f_{leaf}^{-1} \qquad \text{Eq. (7.3.4)}$$

The inverse of f_{leaf} is used, because plants with a lower fraction of leaf tissue are considered to be higher and thus show a higher competitive ability by overtopping other plants. In this way, plants with equal ru_{max} receive equal amounts of resources from one unit of area irrespective of their mass or height in the case of size-symmetric competition, while larger and higher plants receive a higher share of resources in proportion to their shoot geometry in the case of partially asymmetric competition (Schwinning and Parsons, 1999; Weiner et al., 2001). The resource uptake of a plant within one week can then be determined by summing the results of Eq. (7.3..2) over all cells covered by the plant.

To include differences between intra- and interspecific competition, individuals of the same PFT are considered as con-specifics and those of different PFTs as hetero-specifics. The relative competitive ability β_i of one plant is then determined as a decreasing function of the number of plants belonging to the same PFT (n_{PFT}) and covering the same cell:

$$\beta_i = ru_{max} \cdot \frac{1}{\sqrt{n_{PFT}}} \qquad \text{Eq. (7.3.5)}$$

Eq. (7.3.5) is used for size-symmetric competition instead of Eq. (7.3.3). In the case of size asymmetry, plant mass and geometry are taken into consideration according to Eq. (7.3.4). This approach represents a situation where intra-PFT competition is increased relatively to inter-PFT competition and therefore implicitly includes niche differentiation of resource competition at the cell scale, which has been known as an important factor for species coexistence (Chesson, 2000; Silvertown, 2004).

Plant growth and mortality.

Plant growth only depends on the resources (Δres) that the plant acquired during the current time step. In the absence of competition, plants show sigmoid growth. Therefore the growth equation used by Weiner et al. (2001) was adapted to the description of plant geometry used here:

$$\Delta m = g \cdot \left(\Delta res - c_{shoot} \cdot f_{leaf}^{2/3} \cdot ru_{max} \cdot \frac{m_{shoot}^{2}}{m_{max}^{4/3}} \right) \qquad \text{Eq. (7.3.6)}$$

where g is a constant conversion rate between resource units and plant biomass and m_{max} is the maximum mass of shoot and root, respectively. In addition, the maximum amount of resources that is allocated to growth each week is limited by a maximum resource utilization rate given by ru_{max} [resource units/cm²] multiplied by ZOI area [cm²]. If Eq. (B.6) yields a negative result, Δm is set to zero and thus negative growth is prohibited. Lateral plant growth is simulated by considering clonality of plants (see Growth, dispersal and establishment of spacers of clonal plant types).

Growth of generative reproductive mass is restricted to the time between weeks 16 – 21. In this period, a constant fraction of the resources (5 % for all PFTs) is allocated to growth of reproductive mass (Schippers et al., 2001), and reproductive mass is limited to 5 % of shoot mass in total. The same resource conversion rate, g, is used for reproductive and vegetative biomass.

Eqs. (7.3.1) – (7.3.6) are applied to shoot and root ZOIs independently, with the difference that for root growth the factor fleaf is always one. We assume that the minimum uptake of above- and below-ground resources limits plant growth (Lehsten and Kleyer, 2007) and introduced adaptive shoot-root allocation in a way that more resources are allocated to the growth of the plant compartment that harvests the limiting resource (Weiner, 2004). For resource partitioning, we adopt the model of Johnson (1985) which assumes that the fraction of resources allocated to shoot growth is calculated as

$$\alpha_{shoot} = \frac{\Delta res_B}{\Delta res_B + \Delta res_A} \quad \text{Eq. (7.3.7)}$$

where Δres_A is above-ground and Δres_B is below-ground resource uptake.

Plants suffer resource stress if their resource uptake (in any layer) is below a fixed threshold fraction (thr_{res}) of their optimal uptake, which is calculated as maximum resource utilization times ZOI area. That means each week the condition

$\Delta res < thr_{res} * A_{shoot/root} * ru_{max}$

is evaluated and if it is true either for shoot or root the plant is considered as stress exposed during this week, and the state variable "duration of stress exposure", w_{stress}, is incremented. Consecutive weeks of resource stress linearly increase the probability of death

$$p_{mort} = p_{base} + \frac{w_{stress}}{surv_{max}} \quad \text{Eq. (7.3.8)}$$

where $surv_{max}$ is the maximum number of weeks a plant can survive under stress exposure and p_{base} is the stress independent background mortality of 0.7 % per week corresponding to an annual mortality rate of 20 % (Schippers et al., 2001). In order to increase the mean number of PFTs, we extended plant mortality by introducing density dependent background mortality. We multiplied pbase by a density dependent factor:

p_(base_new)=p_base*(1+e^((5*current abundance)/(maximal abundance))) Eq. (7.3.9)

Current abundance is the number of individuals of a PFT existing in the current time step; maximal abundance the potential number of full-grown individuals on the patch in monoculture. A factor of 5 was selected by pattern oriented modelling. Lower factors did not lead to the desired effect of slightly increasing the coexistence/mean number of frequent PFT; higher factors resulted in too strong effects on mortality. Without this extension, plant communities consisted only of 5-6 dominant PFTs. By expert judgement, one would expect a higher number of PFTs in such highly disturbed and nutrient rich environments. By adding that density dependent mortality, mean PFT number increased to 10 frequent

PFTs.

Dead plants do not grow and reproduce anymore, but they still can shade others and are therefore still considered for above-ground competition. Each week the mass of all dead plants is reduced by 50 % and they are removed from the grid completely as soon as their total mass decreases below 10 mg.

Growth, dispersal and establishment of spacers of clonal plant types

For each individual (i.e. ramet) one spacer can grow at a time step. Analogously to generative reproduction, but in each week except for weeks of generative reproduction, 5% of resources acquired by the individual (Δres) are allocated to the growth of the spacer. First, the direction and distance of spacer growth is determined. The direction in which the spacer grows is chosen randomly from a uniform distribution. The distance of spacer growth is randomly chosen from a normal distribution, but the mean distance (SpacerL) is type-specific. The actual distance a spacer grows per week is calculated following:

$$\Delta SpacerL = \Delta res * 0.05 * g \,/\, mSpacer \qquad \text{Eq. (7.3.10)}$$

where g is a constant conversion rate between resource units and plant biomass (see above) and mSpacer is a type unspecific spacer mass of 70 mg per cm; this value was derived as mean of spacer masses of *Phragmites australis* (Granéli et al., 1992) and different sea grass species (Marbà et al., 2002). If the determined distance the spacer has to grow is reached and the respective cell is not the centre of another individual, spacer growth stops and the new ramet can establish with a fixed probability (p_{ram}) (see sub-model “Seed production, dispersal, and establishment” below). If the reached cell is occupied by the centre of a different plant, spacer growth continues randomly within a radius of two cells.

Resource sharing

Clonal plants of the integrator-type (sensu Oborny et al., 2000) share resources throughout the whole genet. Thereby each ramet provides above- and below-ground resources that are not essential for its own survival. The minimum resources (Res_{min}) a ramet needs for survival are calculated as a fixed threshold fraction (thr_{res}) of the ramet´s optimal uptake analogously to the threshold fraction which determines resource stress (see above Plant growth and mortality).

$$Res_{min} = thr_{res} * A_{shoot/root} * ru_{max}. \qquad \text{Eq. (7.3.11)}$$

Surplus resources are added for all ramets of the genet and hence equally shared among ramets. Ramets of non-integrator clonal plant types behave like non-clonal plant individuals in this respect, i.e. they do not share resources.

Seed production, dispersal and establishment

All plants disperse their seeds in week 20 each year. Seed number is determined by dividing reproductive mass by the average mass of one seed (Lehsten and Kleyer, 2007; Schippers et al., 2001). For each seed, dispersal distance is drawn from a log-normal, and direction from a uniform distribution (Stoyan and Wagner, 2001). Note that to avoid edge effects periodic boundary conditions are used.

Germination and seedling establishment are limited to four weeks in autumn directly after dispersal and four weeks in spring of the next year for all PFTs. In between, a winter mortality of 50 % of seeds is assumed and all seeds which did not germinate in these two seasons are removed.

Seedling recruitment is separated in two consecutive processes: (i) Seed germination and (ii) seedling competition. Germination is only allowed in grid cells that are not covered by any plant or its above-ground ZOI. In such cells, seeds germinate with a fixed probability (p_{germ}) and are converted to seedlings. In each cell only a single plant is allowed to establish. Seedling competition is modelled as a weighted lottery, using seed mass as a measure of competitive ability between seedlings (Chesson and Warner, 1981; Schippers et al., 2001). The seedling that is chosen for establishment is converted into a plant with a shoot and root mass equal to seed mass. All other seedlings, which germinated within the cell, die and are removed from the grid.

At the end of the vegetation period all growing spacers of clonal individuals establish with a fixed probability (p_{ram}) unless the cell they have reached by the time is occupied by the centre of a different individual already. If this is the case, the spacer is removed from the grid.

Disturbances

(1) grazing Grazing is modelled as partial removal of an individual's above-ground biomass. The frequency of grazing is specified by a constant weekly probability (p_{graz}) of a grazing event. Grazing is a process that acts selectively towards trait attributes such as shoot size and tissue properties. Therefore, for each plant the susceptibility to grazing (s_{graz}) is calculated as a function of shoot size, geometry and PFT-specific palatability (palat).

$$s_{graz} = m_{shoot} \cdot f_{leaf}^{-1} \cdot palat \qquad \text{Eq. (7.3.12)}$$

The probability for each plant to be grazed within one a grazing event is derived by dividing individual susceptibilities by the current maximum individual susceptibility of all plants. All plants are checked for grazing in random order. In case a plant is grazed, 50 % of its shoot mass and its complete reproductive mass are removed. The random choice of plants is repeated for all other plants until 50 % of the total (aboveground) biomass on the whole grid has been removed. When all plants have been checked for grazing once, but less than 50% of the total above-ground biomass has been removed, grazing probabilities for all individuals are calculated once more based on Eq. (7.3..12) and the whole procedure is repeated until 50% of aboveground biomass has been removed or until a residual biomass is reached which is considered not grazable. This fraction is set to 15 g/m^2 following Schwinning and Parsons (1999). This allows a plant individual to be grazed never or several times during one week with a grazing event.

In addition to stochastic grazing, each year at the end of the vegetation period 50 % of the above-ground mass of all plant individuals is removed to mimic vegetation dieback in winter.

(2) **TRAMPLING** Trampling is integrated to account for effects of crossing vehicles, pedestrians or larger animals. Disturbances related to trampling are subdivided in small patches of 10x10 cm^2 that are randomly distributed on the overall grid. Each week a given percentage of the total area is prone to trampling and plant individuals from the disturbed patches are removed.

(3) **CUTTING** Depending on the management regime, cutting events are simulated one to three times during the vegetation period. During a week of simulated cutting, aboveground biomass of the patch is reduced to 500 mg/m^2. Cutting occurs either in autumn (1 cutting event per year), spring and autumn (2 cutting events per year) or in spring, summer and autumn (3 cutting events per year).

(4) **HERBICIDE EXPOSURE EFFECTS To include effects of herbicide exposure on plant individuals in IBC-grass, we extended the model by toxicological sub-processes. Growth, mortality and establishment of seedlings and adult plants are now influenced by the herbicidal effect rates:**

- **After normal plant growth is calculated, biomass is reduced by the specific effect rate (growthFac):**

  $$m_{shoot} = m_{shoot}*(1\text{-growthFac})$$

  $$m_{root} = m_{root}*(1\text{-growthFac})$$

- **After plants suffered from the stress-induced and/or demographic-related mortali-**

ty, additional herbicide-induced mortality pherb. is included with the specific probabilistic effect rate survFac

- Seedling mortality is increased by the specific probabilistic effect rate survFac
- Seedling biomass is reduced by the specific effect rate growthFacSE after the seedling is established.
- After seeds suffered from the demographic-induced mortality, additional herbicide-induced mortality pherb_SE occurs with the specific probabilistic effect rate survFacSE

In the standard ecotoxicological experiments, effects on dry weight and shoot length are measured (OECD, 2006a, 2006b). However, in IBC-grass we do not consider shoot length directly but indirectly by correlating biomass and growth form in the ZOI approach. In order not to underestimate the effect, we selected the most sensitive endpoint which was dry weight in our case study. Furthermore, in the way we implemented the effects, we cannot relate the effect to the growth rate, which would correspond to the OECD tests, but needed to concentrate the effect into one week. Therefore, effects on biomass can be assumed as very conservative and potentially overestimated.

Effect rates of the herbicides are based on results of standard greenhouse experiments regularly performed for ecotoxicological risk assessments. The resulting dose-response curves are combined with the exposure model Xplicit (Schad and Schulz, 2011; Schad, 2013), which calculates herbicide deposition at varying distances from the field boundary. Here, species effect distributions (SEffDs, effect rate vs. species sensitivity) are calculated for patches at 1-6 meter distance from the arable field. Effective herbicide exposure is considered for one week per year. The described effects on biomass, mortality and establishment are taken from these SEffDs via an http-interface by considering the PFT specific herbicide sensitivity.

REFERENCES

Berendse, F., 1983. Interspecific Competition and Niche Differentiation Between Plantago Lanceolata and Anthoxanthum Odoratum in a Natural Hayfield. J. Ecol. 71, 379. doi:10.2307/2259721

Chesson, P., 2000. Mechanisms of maintenance of species diversity. Annu. Rev. Ecol. Syst. 31, 343–366. doi:10.1146/annurev.ecolsys.31.1.343

Chesson, P.L., Warner, R.R., 1981. Environmental Variability Promotes Coexistence in

Lottery Competitive Systems. Am. Nat. 117, 923. doi:10.1086/283778

Granéli, W., Weisner, S.B., Sytsma, M., 1992. Rhizome dynamics and resource storage in Phragmites australis. Wetl. Ecol. Manag. 1. doi:10.1007/BF00244929

Grimm, V., Berger, U., Bastiansen, F., Eliassen, S., Ginot, V., Giske, J., Goss-Custard, J., Grand, T., Heinz, S.K., Huse, G., Huth, A., Jepsen, J.U., Jørgensen, C., Mooij, W.M., Müller, B., Pe'er, G., Piou, C., Railsback, S.F., Robbins, A.M., Robbins, M.M., Rossmanith, E., Rüger, N., Strand, E., Souissi, S., Stillman, R.A., Vabø, R., Visser, U., DeAngelis, D.L., 2006. A standard protocol for describing individual-based and agent-based models. Ecol. Modell. 198, 115–126. doi:10.1016/j.ecolmodel.2006.04.023

Grimm, V., Berger, U., DeAngelis, D.L., Polhill, J.G., Giske, J., Railsback, S.F., 2010. The ODD protocol: A review and first update. Ecol. Modell. 221, 2760–2768. doi:10.1016/j.ecolmodel.2010.08.019

Johnson, I.R., 1985. A Model of the Partitioning of Growth between the Shoots and Roots of Vegetative Plants. Ann. Bot. 55, 421–431.

Lehsten, V., Kleyer, M., 2007. Turnover of plant trait hierarchies in simulated community assembly in response to fertility and disturbance. Ecol. Modell. 203, 270–278. doi:10.1016/j.ecolmodel.2006.11.034

Marbà, N., Hemminga, M., Mateo, M., Duarte, M., Mass, Y., Terrados, J., Gacia, E., 2002. Carbon and nitrogen translocation between seagrass ramets. Mar. Ecol. Prog. Ser. 226, 287–300. doi:10.3354/meps226287

May, F., Grimm, V., Jeltsch, F., 2009. Reversed effects of grazing on plant diversity: the role of below-ground competition and size symmetry. Oikos 118, 1830–1843. doi:10.1111/j.1600-0706.2009.17724.x

Oborny, B., Kun, a., Czárá, T., Bokros, S., 2000. The effect of clonal integration on plant competition for mosaic habitat space. Ecology 81, 3291–3304. doi:10.1890/0012-9658(2000)081[3291:TEOCIO]2.0.CO;2

OECD, 2006a. Test No. 227: Terrestrial Plant Test: Vegetative Vigour Test, in: OECD Guidelines for the Testing of Chemicals, Section 2. OECD Publishing, Paris.

OECD, 2006b. Test No. 208: Terrestrial Plant Test: Seedling Emergence and Seedling Growth Test, in: OECD Guidelines for the Testing of Chemicals, Section 2. OECD Publishing, Paris.

Schad, T., 2013. Xplicit – A Modelling Framework for Ecological Risk Characterisation at Landscape-scales in Regulatory Risk Assessment and Risk Management of Plant Protection Products.

Schad, T., Schulz, R., 2011. Xplicit, a novel approach in probabilistic spatiotemporally explicit exposure and risk assessment for plant protection products. Integr. Environ. Assess. Manag. 7, 612–23. doi:10.1002/ieam.205

Schippers, P., van Groenendael, J.M., Vleeshouwers, L.M., Hunt, R., 2001. Herbaceous plant strategies in disturbed habitats. Oikos 95, 198–210. doi:10.1034/j.1600-0706.2001.950202.x

Schwinning, S., Parsons, A.J., 1999. The stability of grazing systems revisited: spatial models and the role of heterogeneity. Funct. Ecol. 13, 737–747. doi:10.1046/j.1365-2435.1999.00382.x

Silvertown, J., 2004. Plant coexistence and the niche. Trends Ecol. Evol.

Stoyan, D., Wagner, S., 2001. Estimating the fruit dispersion of anemochorous forest trees. Ecol. Modell. 145, 35–47. doi:10.1016/S0304-3800(01)00385-4

Weiner, J., 2004. Allocation, plasticity and allometry in plants. Perspect. Plant Ecol. Evol. Syst. 6, 207–215. doi:10.1078/1433-8319-00083

Weiner, J., Stoll, P., Muller-Landau, H., Jasentuliyana, A., 2001. The effects of density, spatial pattern, and competitive symmetry on size variation in simulated plant populations. Am. Nat. 158, 438–50. doi:10.1086/321988

Weiß, L., Pfestorf, H., May, F., Körner, K., Boch, S., Fischer, M., Müller, J., Prati, D., Socher, S.A., Jeltsch, F., 2014. Grazing response patterns indicate isolation of semi-natural European grasslands. Oikos 123, 599–612. doi:10.1111/j.1600-0706.2013.00957.x

7.3.3 Additional graphics

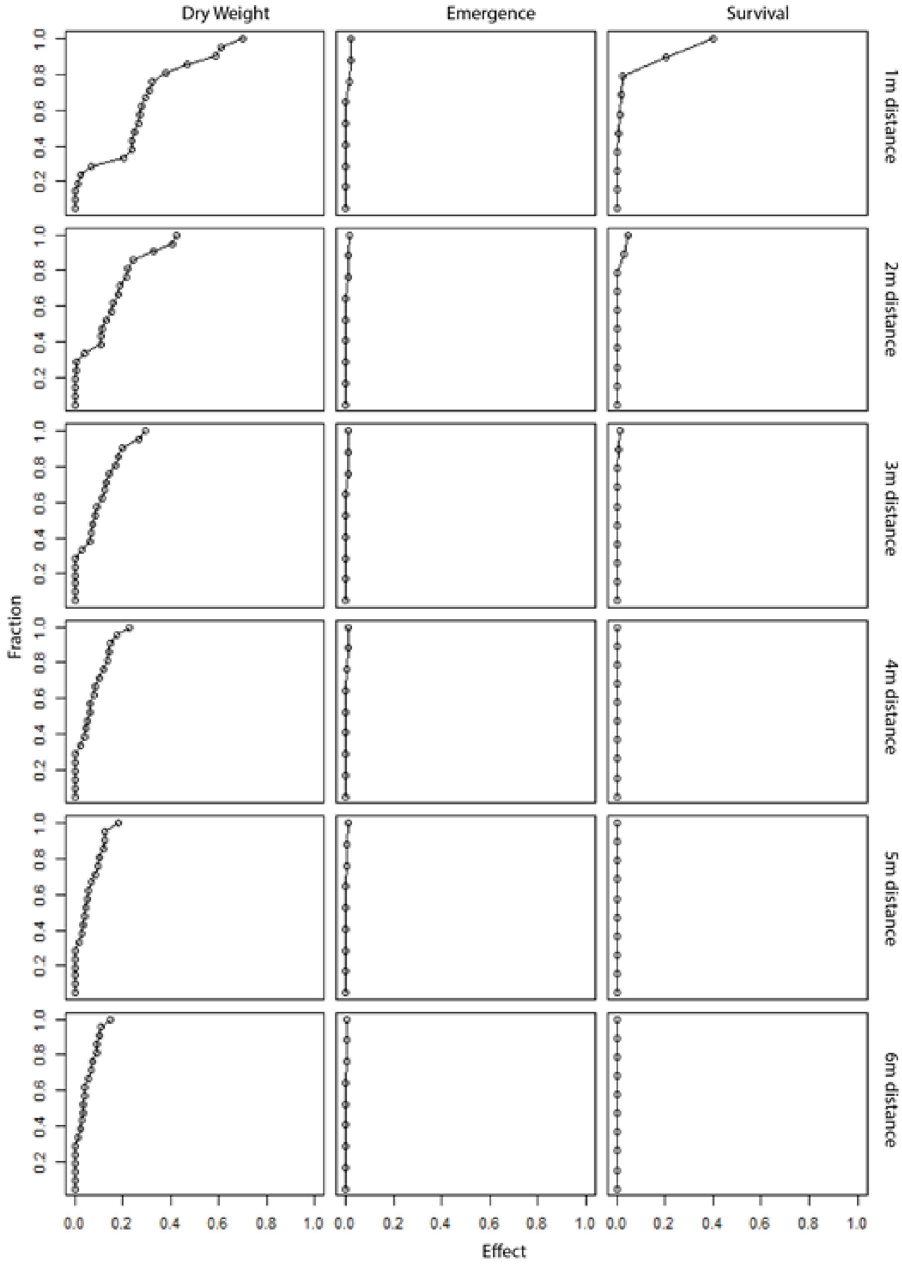

Figure 7.19: Species effect distributions (SEffDs) of the endpoints dry weight, survival and emergence for all simulated patches in 1-6 m distance. SEffDs kept constant over time.

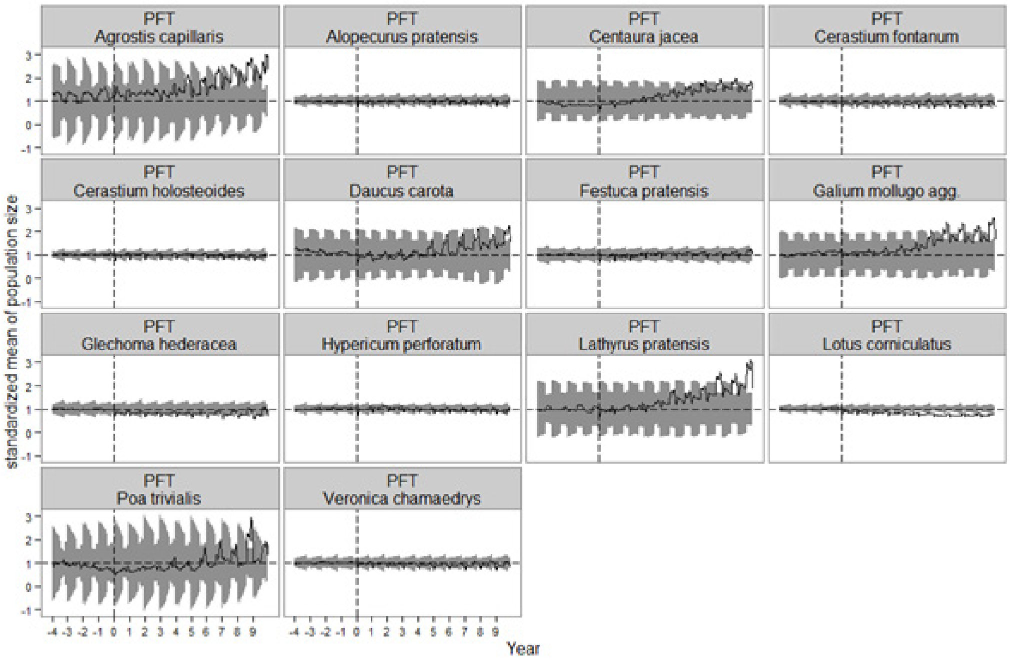

Figure 7.20: Herbicide drift effects on PFT population sizes within community context for field boundary community on a patch in 1m distance. Solid lines represent the standardized mean (standardized by the weekly mean of 50 control simulations) of each week per year out of 50 treatment simulations. A standardized mean of 1 means, that there is no difference between control and treatment. Grey background ribbons showing the standard deviation of standardized control simulations. For a better visualization, only the last 5 years before herbicide drift exposure and 10 years during herbicide exposure and only PFTs with a mean frequency (in control simulations) of >0.9 are presented.

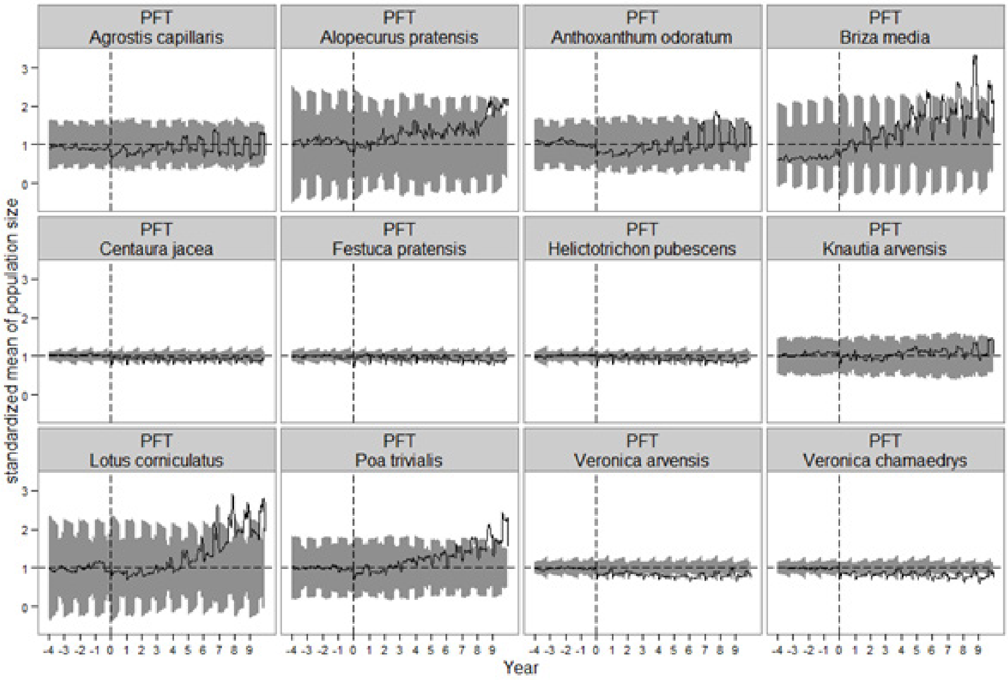

Figure 7.21: Herbicide drift effects on PFT population sizes within community context for *Arrhenatheretalia* community on a patch in 1m distance. Solid lines represent the standardized mean (standardized by the weekly mean of 50 control simulations) of each week per year out of 50 treatment simulations. A standardized mean of 1 means, that there is no difference between control and treatment. Grey background ribbons showing the standard deviation of standardized control simulations. For a better visualization, only the last 5 years before herbicide drift exposure and 10 years during herbicide exposure and only PFTs with a mean frequency (in control simulations) of >0.9 are presented.

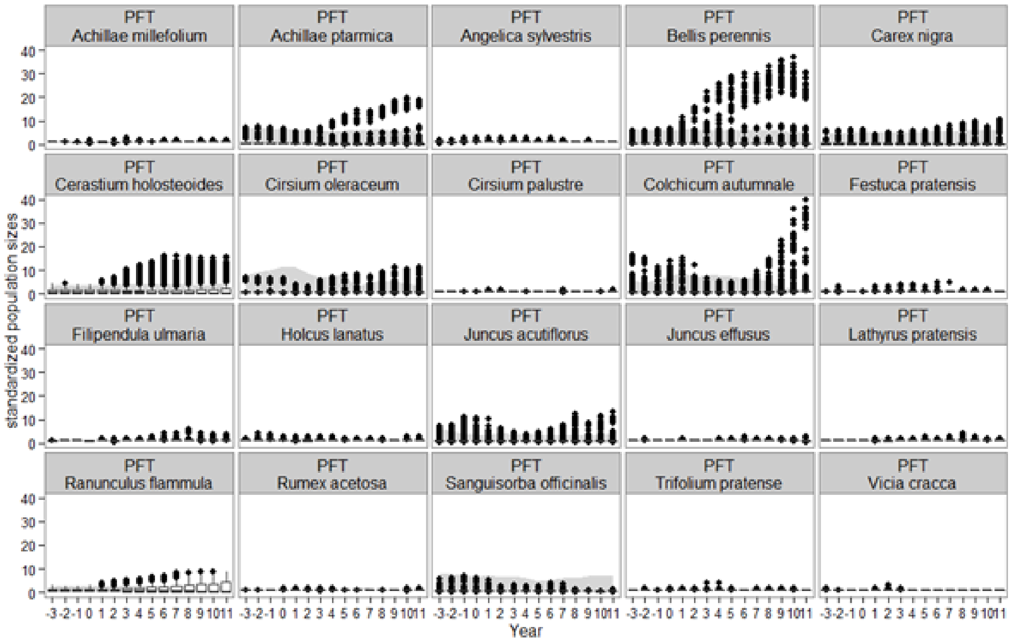

Figure 7.22: Herbicide drift effects on PFT population sizes of infrequent PFTs within community context for *Calthion* community on a patch in 1m distance. Boxplots include the standardized population sizes (by the weekly mean of 50 control simulations) of each week per year out of 50 treatment simulations. A median of 1 means, that there is on average no difference between control and treatment. Grey background ribbons showing the 3rd and 97th percentile of standardized control population sizes. For a better visualization, only the last 3 years before herbicide drift exposure and 11 years during herbicide exposure and only PFTs with a mean frequency (in control simulations) of greater than 0.5 and smaller than 0.9 are presented.

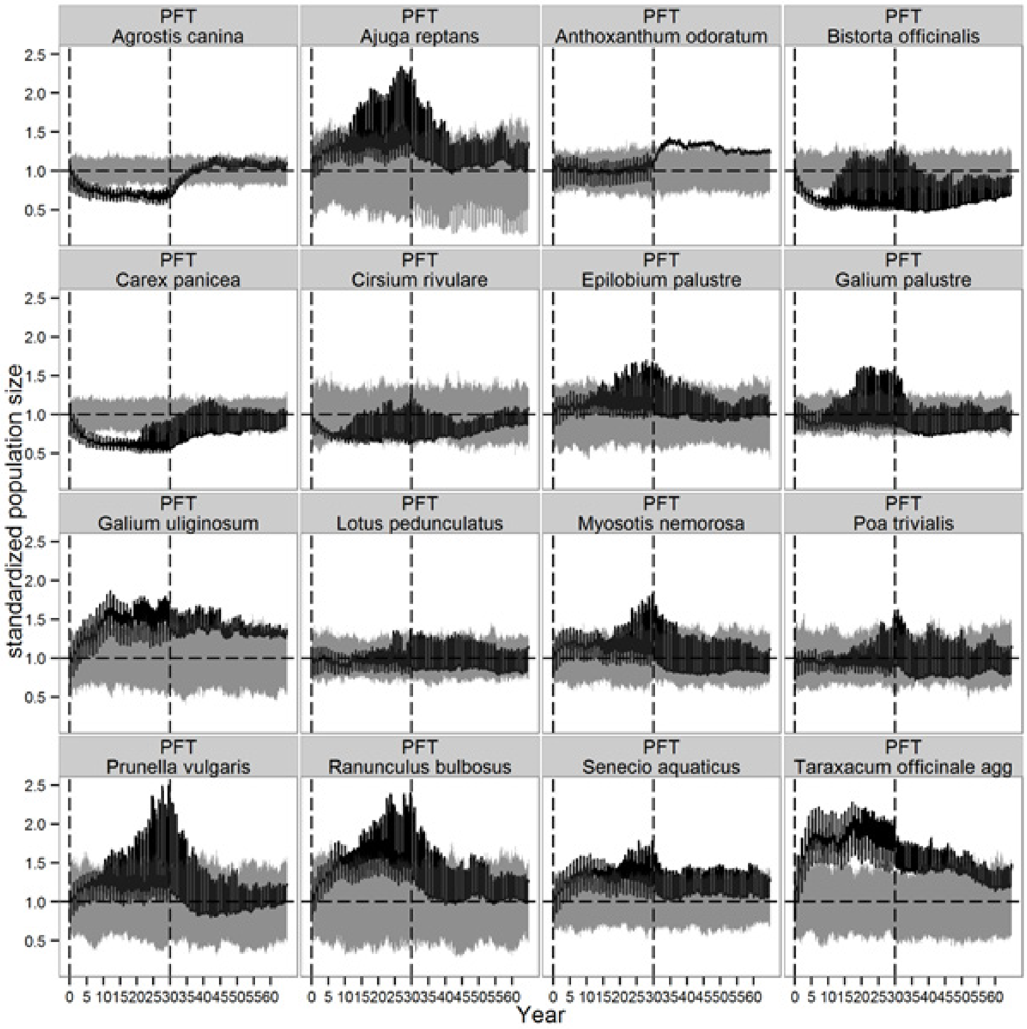

Figure 7.23: **Herbicide drift effects on PFT population sizes within community context for *Calthion* community on a patch in 1m distance.** Solid lines represent the standardized mean (standardized by the weekly mean of 50 control simulations) of each week per year out of 50 treatment simulations. A standardized mean of 1 means, that there is no difference between control and treatment. Grey background ribbons showing the standard deviation of standardized control simulations. During years 0-30 herbicide exposure is simulated followed by 35 years without herbicide exposure to check for recovery potential.

IV Danksagung

Ich möchte mich zunächst bei meinem Hauptbetreuer Florian Jeltsch bedanken. Ohne ihn wäre dieses Projekt erst gar nicht entstanden. Vielen Dank, dass Du mir die Möglichkeit gegeben hast in diesem Projekt zu arbeiten und meine Doktorarbeit zu schreiben. Vielen Dank für Dein konstruktives Feedback und die anregenden Diskussionen während der letzten Jahre.

Ich danke der Bayer AG, die dieses Projekt finanziert hat. Außerdem danke ich meinen Kollegen und Kolleginnen von Bayer, Thorsten Schad, Thomas Preuss, Simon Heine, Christine Mihan, Andreas Solga und Sean McGee, für die ausgiebigen Diskussionen und vielen Ideen, die wir in den letzten Jahren umsetzen konnten.

Ich möchte mich außerdem bei allen bedanken, mit denen ich in den letzten Jahren mein Büro geteilt habe: Danke Sebastian, dass ich immer meine Sorgen und Probleme mit dir teilen konnte und du immer ein offenes Ohr hast! Danke an Lisa, Merlin und Katrin, dass ich euch jederzeit von eurer Arbeit abhalten konnte, wenn ich Fragen hatte!

Außerdem möchte ich mich auch bei sämtlichen Mitgliedern der AG bedanken, die mich teilweise schon seit meiner Masterarbeit begleitet haben. Besonderer Dank geht an Michael, Kolja und Katja, dafür dass ich mich bei pflanzenspezifischen Fragen an euch wenden konnte.

Natürlich möchte ich auch meinem Zweitbetreuer, Volker Grimm, danken, der mich besonders in den letzten Zügen unterstützt hat.

Zu guter Letzt möchte ich mich bei meinen Eltern bedanken, die mich immer unterstützt haben und mich meinen eigenen Weg haben finden lassen. Ich bin auch meiner Schwester und meinen Freunden dankbar, dass sie immer ein offenes Ohr hatten und mich in stressigen Situationen beruhigt haben.

V Declaration

I herewith declare that I independently and with the help of my supervisors prepared this dissertation. My cumulative dissertation consists of three peer-reviewed publications. The second chapter of my thesis is published in Environmental Sciences Europe (2018), the third chapter is published in Environmental Toxicology and Chemistry (2018) and the fourth chapter is published in Ecological Modelling (2017). I am the first author of all publications. With the support of my co-authors I developed the research questions and study designs. I implemented the extensions in the model, parameterized the model and ran all model simulations on my own. I was also responsible for data analyses and the writing of the manuscript. My coauthors supported me in interpreting the results and writing the manuscripts.

I did not use any sources other than those specified in the list of references. All parts, which originate literally or meaningfully from other sources, are marked as such.

This thesis has not been submitted to any other university of examination board before.

Potsdam, 18.01.2019

Jette Reeg