



# Modelling the Spatial Variation in *Alopecurus myosuroides* for Precision Weed Management

Submission of thesis for the degree of PhD in Agriculture

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# Abstract

*Alopecurus myosuroides* Huds. (black-grass) grows in patches within fields. This presents an opportunity for site-specific management by patch spraying. Despite the economic and environmental benefits of this type of management, it is not being readily taken up by farmers, largely due to the risk of missing weeds that fall outside of established patches. I focus on the environmental determinants of patch location in *A. myosuroides* and the scale-dependence of relationships between *A. myosuroides* and environmental properties. Understanding these relationships allowed me to determine which abiotic factors can be used to identify *A. myosuroides* vulnerable zones within fields and if these relationships occur at scales appropriate for management. This presents a more conservative approach than patch spraying according to observations of previous years' infestations, as a greater area of the field is sprayed, yet the overall use of pesticide is still reduced.

By combining field work, pot experiments, and modelling, I discovered that soil organic matter, water, and pH, amongst other environmental properties, show strong scale-dependent relationships with the within-field distribution of *A. myosuroides*. These relationships between *A. myosuroides* and soil properties were often strongest at coarse scales making them particularly useful for the implementation of management practices, which are often limited to coarse-scale implementation by the available machinery. The effects of these soil properties on *A. myosuroides* are both direct (affecting the plant's life-cycle) and indirect (altering herbicide efficacy). The incremental changes I observed to different aspects of the life-cycle due to soil properties may seem too small to be of consequence when studied independently, yet when combined in a modelling approach their additive nature revealed them as important determinants of the within-field distribution of this species and the coarse-scale relationships observed in the field are an emergent property of the model.

# Declaration of original authorship

I confirm that this is my own work and the use of all material from other sources has been properly and fully acknowledged.

Helen Metcalfe

# Contribution to jointly authored papers

Included in this thesis are published papers and papers submitted for publication. These papers are written by multiple authors and as such I use the plural pronoun “we” when referring to who did the work, elsewhere in the thesis where the work is entirely my own I use the singular “I”. I can confirm that I am the lead author of each and have made a substantial contribution to each of the papers included. Each of these papers is detailed below with an estimation of each author’s contribution to the conception, initiation and planning, execution, and preparation of the manuscript outlined in Table i.

Chapter 2 consists largely of the following published paper: Metcalfe H, Milne AE, Webster R, Lark RM, Murdoch AJ, Storkey J, 2016. Designing a sampling scheme to reveal correlations between weeds and soil properties at multiple spatial scales. *Weed Research*, **56** (1) 1–13.

Chapter 3 consists largely of the following paper under review with Weed Research: Metcalfe H, Milne AE, Webster R, Lark RM, Murdoch AJ, Kanelo L, Storkey J, 2017. Defining the habitat niche of black-grass (*Alopecurus myosuroides*) at the field scale. Submitted to *Weed Research*.

Chapter 4 consists in part of the following published paper: Metcalfe H, Milne AE, Murdoch AJ, Storkey J, 2017. Does variable soil pH have an effect on the within-field distribution of *A. myosuroides*? *Aspects of Applied Biology* **134** 145–150.

Chapter 5 consists largely of the following paper under review with Pest Management Science: Metcalfe H, Milne AE, Hull R, Murdoch AJ, Storkey J, 2017. The implications of spatially variable pre-emergence herbicide efficacy for weed management. Submitted to *Pest Management Science*.

**Table i.** Contribution of authors to each of the included papers

Author	Percentage contribution		
	Conception, initiation and planning	Execution	Preparing the manuscript
<i>Designing a sampling scheme to reveal correlations between weeds and soil properties at multiple spatial scales.</i>			
<b>Metcalfe H</b>	<b>10</b>	<b>35</b>	<b>75</b>
Milne AE	30	15	5
Webster R	5	15	5
Lark RM	5	15	5
Murdoch AJ	10	5	5
Storkey J	30	15	5
<i>Defining the habitat niche of black-grass (<i>Alopecurus myosuroides</i>) at the field scale.</i>			
<b>Metcalfe H</b>	<b>46</b>	<b>64</b>	<b>76</b>
Milne AE	20	10	5
Webster R	2	4	5
Lark RM	5	4	5
Murdoch AJ	5	4	2
Kanelo L	2	10	2
Storkey J	20	4	5
<i>Does variable soil pH have an effect on the within-field distribution of <i>A. myosuroides</i>?</i>			
<b>Metcalfe H</b>	<b>50</b>	<b>55</b>	<b>85</b>
Milne AE	5	10	5
Murdoch AJ	5	5	5
Storkey J	40	30	5
<i>The implications of spatially variable pre-emergence herbicide efficacy for weed management</i>			
<b>Metcalfe H</b>	<b>70</b>	<b>55</b>	<b>80</b>
Milne AE	5	5	5
Hull R	10	30	5
Murdoch AJ	5	5	5
Storkey J	10	5	5

# Contents

Acknowledgements . . . . .	i
Abstract . . . . .	ii
Declaration of original authorship . . . . .	iii
<b>1 Introduction</b>	<b>2</b>
1.1 Weed Management . . . . .	5
1.1.1 Site-Specific Weed Management . . . . .	7
1.2 Within-Field Spatial Heterogeneity in Weed Distributions . . . . .	11
1.2.1 Weed Biology and Ecology . . . . .	12
1.2.2 Agronomy . . . . .	14
1.2.3 Environment . . . . .	15
1.3 Objectives . . . . .	17
1.3.1 Hypotheses . . . . .	18
1.4 References . . . . .	20
<b>2 Designing a Sampling Scheme to Reveal Correlations Between Weeds and Soil Properties at Multiple Spatial Scales</b>	<b>27</b>
2.1 Summary . . . . .	28
2.2 Introduction . . . . .	29
2.3 Materials and Methods . . . . .	31
2.3.1 Study Site . . . . .	31
2.3.2 Sampling Scheme . . . . .	31
2.3.3 Soil Analyses . . . . .	37
2.3.4 Statistical Analyses . . . . .	37
2.4 Results . . . . .	39
2.4.1 Optimizing the Design . . . . .	48
2.5 Discussion and Conclusions . . . . .	50
2.6 Acknowledgements . . . . .	52

2.7	References . . . . .	53
<b>3</b>	<b>Defining the Habitat Niche of Black-grass (<i>Alopecurus myosuroides</i>) at the Field Scale.</b>	<b>56</b>
3.1	Summary . . . . .	57
3.2	Introduction . . . . .	58
3.3	Materials and Methods . . . . .	61
3.3.1	Field Sites . . . . .	61
3.3.2	Nested Sampling . . . . .	61
3.3.3	Weed Counts . . . . .	63
3.3.4	Soil Analyses . . . . .	63
3.3.5	Topography . . . . .	64
3.3.6	Analysis . . . . .	64
3.4	Results . . . . .	66
3.4.1	Variograms and Kriging . . . . .	69
3.4.2	Principal Components Analysis . . . . .	72
3.4.3	Nested Analysis . . . . .	72
3.4.4	Regression analysis . . . . .	76
3.5	Discussion . . . . .	78
3.5.1	Conclusions . . . . .	80
3.6	Acknowledgements . . . . .	80
3.7	References . . . . .	81
<b>4</b>	<b>The Effect of the Abiotic Environment on the Life-Cycle of Black-grass (<i>Alopecurus myosuroides</i>)</b>	<b>84</b>
4.1	Summary . . . . .	85
4.2	Introduction . . . . .	86
4.3	Methods . . . . .	89
4.3.1	Plant material . . . . .	89
4.3.2	Experiment 1: Soil Organic Matter and Water Input . . . . .	89
4.3.3	Experiment 2: pH . . . . .	92
4.3.4	Experiment 3: pH and Crop Competition . . . . .	92
4.3.5	Data Analysis . . . . .	94
4.4	Results . . . . .	94
4.4.1	Experiment 1: Soil organic matter and water input . . . . .	94

4.4.2	Experiment 2: pH . . . . .	100
4.4.3	Experiment 3: pH and crop competition . . . . .	100
4.5	Discussion . . . . .	103
4.6	Conclusions . . . . .	105
4.7	References . . . . .	106
<b>5</b>	<b>The Implications of Spatially Variable Pre-Emergence Herbicide Efficacy for Weed Management</b>	<b>108</b>
5.i	Preliminary Methods . . . . .	109
5.ii	Preliminary Results . . . . .	111
5.1	Summary . . . . .	113
5.2	Introduction . . . . .	114
5.3	Methods . . . . .	116
5.3.1	Soils . . . . .	116
5.3.2	Plant Material . . . . .	118
5.3.3	Pre-emergence Herbicides . . . . .	118
5.3.4	Herbicide Efficacy . . . . .	119
5.3.5	Sub-lethal Effects . . . . .	119
5.3.6	Data Analysis . . . . .	120
5.3.7	Modelling . . . . .	120
5.4	Results . . . . .	123
5.4.1	Modelling . . . . .	130
5.5	Discussion . . . . .	134
5.6	Acknowledgements . . . . .	138
5.7	References . . . . .	139
<b>6</b>	<b>Modelling the Spatial Variation in Black-grass (<i>Alopecurus myosuroides</i>) due to Soil Properties</b>	<b>142</b>
6.1	Summary . . . . .	143
6.2	Modelling weed population dynamics . . . . .	143
6.2.1	Life-cycle Models . . . . .	146
6.2.2	Spatial Structure in population dynamics . . . . .	148
6.2.3	Environment . . . . .	149
6.3	Introduction . . . . .	149
6.3.1	Objectives . . . . .	151

6.4	Model Implementation . . . . .	151
6.4.1	Soil Properties . . . . .	155
6.4.2	Management . . . . .	156
6.4.3	<i>A. myosuroides</i> Emergence . . . . .	157
6.4.4	Herbicide Mortality . . . . .	161
6.4.5	Seed Production . . . . .	163
6.4.6	Seed Losses . . . . .	166
6.4.7	Seed Dispersal . . . . .	166
6.4.8	Vertical Movement of Seed in the Soil . . . . .	168
6.5	Model Validation . . . . .	169
6.5.1	Patch Location . . . . .	169
6.5.2	Scale-dependent Correlations . . . . .	169
6.6	Results . . . . .	171
6.6.1	Patch Location . . . . .	171
6.6.2	Scale-dependent Correlations . . . . .	177
6.7	Discussion . . . . .	181
6.7.1	Conclusions . . . . .	183
6.8	Acknowledgements . . . . .	184
6.9	References . . . . .	184
<b>7</b>	<b>Discussion</b>	<b>191</b>
7.1	Recommendations for Further Research . . . . .	200
7.1.1	Improving the understanding of the within-field spatial distribu- tion of <i>A. myosuroides</i> . . . . .	202
7.1.2	Within-field spatial patterns of herbicide resistance . . . . .	202
7.1.3	Development of the mechanistic model to identify weed vulnera- ble zones . . . . .	204
7.2	References . . . . .	205
	Bibliography . . . . .	206
	<b>Supplementary Material</b>	<b>222</b>

# List of Figures

1.1	Mean long-term winter wheat grain yields on the Broadbalk long-term experiment at Rothamsted. . . . .	3
1.2	<i>Alopecurus myosuroides</i> plant in a crop of winter wheat. . . . .	5
1.3	Diagrammatic representation of the principles of patch spraying. . . . .	9
1.4	The life-cycle of <i>A. myosuroides</i> . . . . .	12
2.1	Example of a balanced nested sampling design and topological tree. . . . .	33
2.2	Location of sampling points within the field in Harpenden. . . . .	35
2.3	Nested sampling design and topological tree used in the field in Harpenden. . . . .	36
2.4	Accumulated components of variance and variograms for selected measured variables in the field in Harpenden. . . . .	42
2.5	Kriged map of <i>A. myosuroides</i> in the field in Harpenden. . . . .	43
2.6	Kriged maps of soil properties in the field in Harpenden. . . . .	45
2.7	Scale-dependent correlations between <i>A. myosuroides</i> and soil properties in the field in Harpenden. . . . .	47
2.8	Optimized nested sampling designs. . . . .	49
3.1	Nested sampling designs used in field studies. . . . .	62
3.2	Sampling locations, seedling and head counts in each of the five fields. . . . .	72
3.3	Principal component analysis on soil properties measured in four study sites. . . . .	73
3.4	Scatter plots showing the relationship between the observed <i>A. myosuroides</i> seedling densities and the values predicted by the regression model. . . . .	77
3.5	Scatter plots showing the relationship between the observed <i>A. myosuroides</i> head counts and the values predicted by the regression model. . . . .	78
4.1	The life-cycle of <i>A. myosuroides</i> . . . . .	88
4.2	Configuration of plants within pots. . . . .	93

4.3	Germination over time in Experiment 1. . . . .	95
4.4	Germination over hydrothermal time in Experiment 1. . . . .	96
4.5	The height of <i>A. myosuroides</i> plants grown in trial one at two different levels of water input. . . . .	98
4.6	The number of seed heads per <i>A. myosuroides</i> plant grown in trial one at two different levels of water input. . . . .	99
4.7	Germination data with separate curves fitted for each soil pH. . . . .	101
4.8	The relative biomass of wheat and <i>A. myosuroides</i> plants grown in competition compared to when grown in isolation. . . . .	103
5.i	Proportion of seedlings surviving eight weeks after the application of pre-emergence herbicides. . . . .	112
5.1	The proportion of seedlings surviving six weeks after the application of two pre-emergence herbicides on soil with varying levels of organic matter. . . . .	125
5.2	The log dry weight of seedlings surviving six weeks after the application of two pre-emergence herbicides on soil with varying levels of organic matter. . . . .	127
5.3	The total dry weight of mature plants after the application of two pre-emergence herbicides on soil with varying levels of organic matter. . . . .	130
5.4	Weed seed production in the absence and presence of crop competition. . . . .	133
6.1	Basic component structure of the spatially explicit life-cycle model of within-field <i>A. myosuroides</i> population dynamics. . . . .	155
6.2	Germination data plotted against hydrothermal time. . . . .	160
6.3	Relationship between soil organic matter and survival after the application of pre-emergence herbicide. . . . .	162
6.4	Density dependent relationship between plants and heads. . . . .	164
6.5	Relationship between soil organic matter and the number of heads per plant. . . . .	165
6.6	Numerical order of assessment of nearby squares for the dispersal of seeds from a plant in the centre square. . . . .	167
6.7	Maps showing the kriged log seedling counts and model output for each field. . . . .	176
6.8	Frequency distribution of correlation coefficients between model simulations and kriged log seedling counts for each field. . . . .	176

6.9	Frequency distribution of P values associated with correlation coefficients shown in Figure 6.8. . . . .	176
6.10	Frequency distribution of scale-dependent correlation coefficients between the simulated number of <i>A. myosuroides</i> seedlings and simulated soil properties used as inputs into the model simulations for the field in Harpenden. . . . .	181
6.11	Frequency distribution of scale-dependent correlation coefficients between the simulated number of <i>A. myosuroides</i> seedlings and simulated soil properties used as inputs into the model simulations for the field in Haversham. . . . .	181
7.1	Diagrammatic representation of the principles of patch spraying. . . . .	201
7.2	Results of resistance assay to pendimethalin in the Harpenden field. . . . .	203
S3.1	Maps showing the kriged soil moisture content measured by loss on ignition in each of the five fields. . . . .	227
S3.2	Maps showing the kriged soil organic matter measured by loss on ignition in four fields. . . . .	227
S3.3	Maps showing the kriged soil clay content measured by loss on ignition in each of the five fields. . . . .	227
S3.4	Maps showing the kriged soil pH measured by loss on ignition in each of the five fields. . . . .	227
S5.1	The number of tillers per plant surviving six weeks after the application of two pre-emergence herbicides on soil with varying levels of organic matter. . . . .	237
S5.2	Outputs from 100 simulations for each of 10 years of weather data from the INTERCOM model. . . . .	237
S6.1	Frequency distribution of scale-dependent correlation coefficients between the simulated number of <i>A. myosuroides</i> heads and simulated soil properties in Harpenden. . . . .	241
S6.2	Frequency distribution of scale-dependent correlation coefficients between the simulated number of <i>A. myosuroides</i> heads and simulated soil properties in Haversham. . . . .	241

# List of Tables

i	Contribution of authors to each of the included papers . . . . .	v
2.1	Summary statistics of species counts and environmental variables in the field in Harpenden. . . . .	40
2.2	Variogram models fitted to describe the spatial structure in selected measured variables in the field in Harpenden. . . . .	42
2.3	Estimated variance components for environmental variables and <i>A. myosuroides</i> at multiple spatial scales. . . . .	45
2.4	Pearson correlation coefficients between <i>A. myosuroides</i> counts and soil properties measured taking all data into account. . . . .	48
2.5	Results of REML analysis for log transformed <i>A. myosuroides</i> counts. . . . .	49
3.1	Scales used at each level of the nested sampling design in each field. . . . .	62
3.2	Summary statistics for <i>A. myosuroides</i> counts and soil properties. . . . .	67
3.3	Pearson correlation coefficients between <i>A. myosuroides</i> counts and soil properties. . . . .	71
3.4	Scale-dependent correlations between <i>A. myosuroides</i> counts and soil properties. . . . .	74
3.5	Terms selected in a regression type analysis using REML to predict <i>A. myosuroides</i> seedling densities from soil properties. . . . .	77
4.1	The volumetric composition, measured soil organic matter, and pH of the soil mixtures. . . . .	91
4.2	Parameters of the Gompertz model for germination in Experiment 1. . . . .	95
4.3	Summary of data for the day of first flowering in Experiment 1. . . . .	97
4.4	Parameters of the Gompertz model for germination in Experiment 2. . . . .	100
4.5	Summary of data for the day of first flowering in Experiment 2. . . . .	101
4.6	Summary of data for the height of the tallest tiller. . . . .	102

5.i	Application rates of two pre-emergence herbicides in the preliminary investigation. . . . .	110
5.1	The volumetric composition, measured soil organic matter, and pH of the soil mixtures. . . . .	117
5.2	The models considered for describing the dose-response relationships. . . . .	121
5.3	Fitted parameter values for the Cedergreen-Ritz-Streibig model used to describe <i>A. myosuroides</i> survival. . . . .	123
5.4	Fitted parameter values for the log-logistic model used to describe <i>A. myosuroides</i> biomass. . . . .	127
5.5	The number of seed heads and the dry weight of that seed. . . . .	128
5.6	The predicted proportion of seedlings surviving and the dry weight of those seedlings surviving six weeks after the application of either flufenacet or pendimethalin on soil with varying levels of organic matter. . . . .	131
5.7	The predicted ED50 for seedling survival, seedling biomass and weed seed production. . . . .	135
6.1	Nomenclature used in Chapter 6. . . . .	152
6.2	Starting conditions used to check suitability of equations in Section 6.4.3 for modelling germination rates. . . . .	159
S3.1	Terms selected in a regression type analysis using REML to predict <i>A. myosuroides</i> head densities from soil properties. . . . .	222
S4.1	ANOVA table for the total number of seeds germinating in Experiment 1, Chapter 4. . . . .	228
S4.2	Non-linear regression analysis to fit a Gompertz curve to germination data collected in Experiment 1, Chapter 4. . . . .	229
S4.3	ANOVA table for the Julian day of first flowering in Experiment 1, Chapter 4. . . . .	229
S4.4	ANOVA table for the height of the plants at maturity in Experiment 1, Chapter 4. . . . .	229
S4.5	ANOVA table for the number of seed heads per plant at maturity in Experiment 1, Chapter 4. . . . .	230
S4.6	ANOVA table for the total dry weight of seed heads at maturity in Experiment 1, Chapter 4. . . . .	230

S4.7 ANOVA table for the total dry weight of seed heads at maturity in Experiment 1, Chapter 4. . . . .	230
S4.8 ANOVA table for the total dry weight of seed heads at maturity in Experiment 1, Chapter 4. . . . .	231
S4.9 ANOVA table for the total number of seeds germinating in Experiment 2, Chapter 4. . . . .	231
S4.10 Non-linear regression analysis to fit a Gompertz curve to germination data collected in Experiment 1, Chapter 4. . . . .	231
S4.11 ANOVA table for the Julian day of flowering in Experiment 3, Chapter 4.	232
S4.12 ANOVA table for the height of plants in Experiment 3, Chapter 4. . . . .	232
S4.13 ANOVA table for the number of seed heads in Experiment 3, Chapter 4. . . . .	233
S4.14 ANOVA table for the dryweight of seed heads in Experiment 3, Chapter 4.	233
S4.15 ANOVA table for the total plant dryweight in Experiment 3, Chapter 4. . . . .	234
S4.16 ANOVA table for the relative biomass of plants when grown in competition to when grown in isolation in Experiment 3, Chapter 4. . . . .	234
S5.1 Fitted parameter values for the log-logistic model used to describe <i>A. myosuroides</i> tiller numbers. . . . .	235

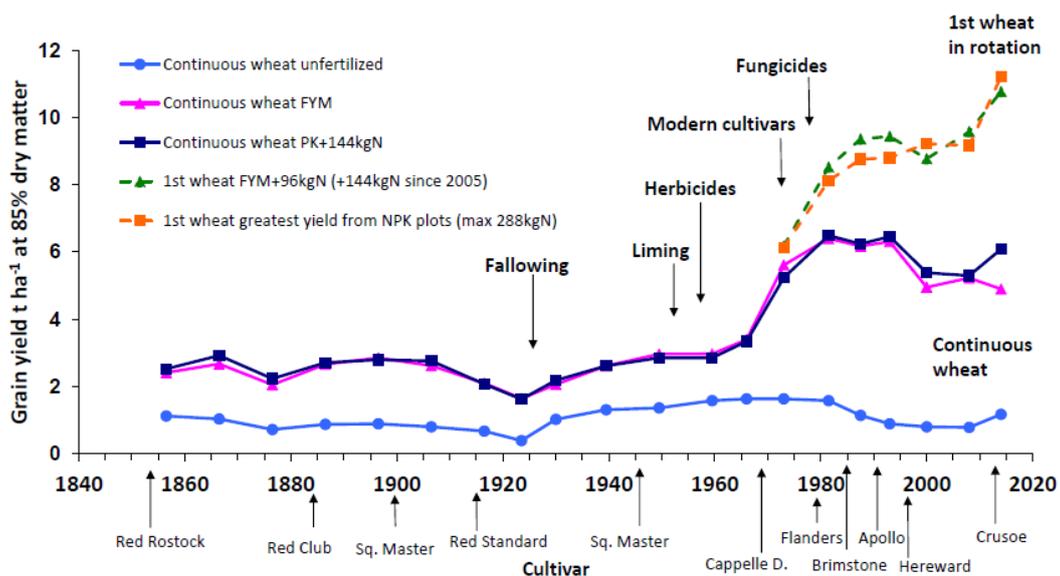
# Chapter 1

## Introduction

In a world where the population is set to reach 9.7 billion in 2050 (UN, DESA, 2015), food security is an issue of great importance. The severity of this issue is recognized in the United Nations' sustainable development goals (UN, 2017). These not only encompass zero hunger, but also good health and well-being, sustainable cities and communities, responsible consumption and production, and climate action. Each of these goals requires forward steps in the field of food security in order to be achieved. In the global efforts to realise these goals, not only does food production need to increase, but this needs to be done in a more sustainable, climate-friendly manner, using less land and ensuring the foods we produce are healthy.

The Green Revolution of the 1950s, 1960s and 1970s saw the widespread uptake of agricultural technologies including irrigation, pesticides and synthetic nitrogen fertilisers. It also saw the introduction of improved crop varieties, bred to include semi-dwarfing genes. These lead to improved yields and an improved harvest index by allowing extra nitrogen uptake by the plant whilst reducing the risk of lodging. These combined improvements to agricultural practice and technologies allow increased production across all crops, with cereal yield worldwide increasing by more than 50% over the period 1961-1981 (FAOSTAT, 2017). These yield increases, and the technologies that allowed them, are exemplified in the Broadbalk experiment at Rothamsted Research (Figure 1.1) where winter wheat has been sown and harvested on all or part of the field each year since 1983, making it the longest continuously running agronomic experiment in the world. Key agronomic changes introduced throughout the Green Revolution were also introduced into this experiment and so the changing yield observed provides a good

indication of the advantages provided by each subsequent technological or agronomic advancement (Figure 1.1). Particularly striking is the yield increase following the introduction of herbicides and the first modern short-strawed variety “Capelle D.” These combined improvements in cultivars and increased agricultural inputs, demonstrated in this experiment, underpinned the yield increases observed during the Green Revolution. Following these improvements made during the Green Revolution yield increases have begun to stagnate with an increasing gap between potential yields and those achieved on farms — the so-called “yield gap”. This indicates that the technological advances of the Green Revolution can no longer be relied upon to support yield gains and instead we should now be aiming to improve the efficiency of resource use and production, for example by integrating ecology with food production to reduce the need for external inputs (Smith *et al.*, 2010).



**Figure 1.1.** Mean long-term winter wheat grain yields on the Broadbalk long-term experiment at Rothamsted. The introduction of new wheat varieties to the experiment are shown beneath the x-axis. The timing of the introduction of new agricultural practices are indicated by arrows. This image is licensed under a Creative Commons Attribution 4.0 International Licence - Rothamsted Research 2017.

Cereals make up the majority of production in the crop sector and are the most important food source for human consumption (FAO, 2015). The Food and Agriculture Organization of the United Nations (FAO, 2017) estimates world cereal production in 2016 to have amounted to 2,600 million tonnes. In the United Kingdom (UK), 51%

of the 6.1 million-hectare croppable area was in cereal production in 2015 making cereals a key aspect of the UK agricultural industry (National Statistics, 2015). These statistics highlight the importance of cereals in our food system. Therefore, in order to meet global food security challenges there is not only a need to improve the yield and nutritional value of cereals but also to minimize the yield gap associated with their production.

Weeds affect crop productivity through competition for resources; water, light, and inorganic nutrients. They are the largest single crop protection limitation on crop yield worldwide (Ziska & Dukes, 2011) and are the most important pest group in wheat production, causing potential losses of 23%, compared to only 16, 3, and 9% for pathogens, viruses, and animal pests respectively (Oerke, 2006). As such they are a major limitation on food production and present an important obstacle if we are to achieve the sustainable development goals relating to food security outlined above. They are also of huge economic importance. A weed can be defined as a plant growing out of place (Radosevich *et al.*, 2007 p4). In agriculture, this translates as plants other than the crop being grown for commercial production. This can include both wild plants that establish within the agricultural landscape as well as volunteers from previous crops. Weeds often exhibit rapid vegetative growth and are able to germinate, grow and reproduce in a wide range of environments (Baker, 1974). They are also very quick to adapt to changing selection pressures (Neve *et al.*, 2009). This makes them very difficult to manage in an agricultural situation as they can quickly adapt to changing management practices.

*Alopecurus myosuroides* Huds. (black-grass), an annual grass, is one of the most common grass weeds of winter cereals in north-west Europe (Holm *et al.*, 1997) and is particularly problematic in the UK (Figure 1.2). *Alopecurus myosuroides* produces many seeds and shows strong competitive ability with the crop (Maréchal *et al.*, 2012). The distribution of the species within the UK corresponds primarily to that of the wheat growing area and is largely concentrated in the south and east. With climate change the distribution of *A. myosuroides* is predicted to remain broadly similar with a possible northward shift in its range (Stratonovitch *et al.*, 2012). *Alopecurus myosuroides* exhibits two cohorts of germination; the majority of seedlings emerge in the autumn, and a second smaller flush in the spring. By emerging whilst the crop is in the field, there is synchronisation with the crop life-cycle allowing it to compete at all stages of growth

(Maréchal *et al.*, 2012), whilst completing its life-cycle before the crop is harvested. Seed shed occurs from late June to mid August with peak shedding occurring in late July (Moss, 1980). *Alopecurus myosuroides* plants are capable of producing vast amounts of seeds (Moss, 1980), meaning small failures in control can lead to rapid population growth and dense infestations within some fields. As such, control of their population is of great importance to farmers.



**Figure 1.2.** *Alopecurus myosuroides* plant in a crop of winter wheat. This image is licensed under a Creative Commons Attribution 4.0 International Licence - Rothamsted Research 2017.

## 1.1 Weed Management

The first chemicals used for weed control were introduced in the early 1900s, but it was in the 1940s that the development of new herbicides dramatically increased farmers' ability to control weeds (Oerke, 2006). For many farmers, the main option for control of *A. myosuroides* and other weeds is still through the application of herbicides. These are often heavily relied upon as the sole method of control and are generally applied using a broadcast spray. In 2015, in the UK, 4,200 tonnes of herbicide were applied to cereal crops (FERA, 2017) with farmers using an average of six herbicidal active substances in a season for a single arable crop (Garthwaite *et al.*, 2014). For *A. myosuroides*, herbicides have long proven to be effective at killing individuals as well as suppressing growth and seed return of survivors (Moss, 1980), yet many farmers are seeing a decline in the levels of control achieved as *A. myosuroides* populations in the UK are rapidly developing resistance to many commonly used active ingredients including acetyl-CoA carboxylase

(ACCase) and acetolactate synthase (ALS) type herbicides (Heap, 2017) and so farmers are looking to find alternative methods of weed management.

There are also economic, environmental and legislative pressures on the use of herbicides. First, the cost of agrochemicals, whilst small, is an important component in the cost of cereal production. Second, there are many environmental concerns surrounding the widespread use of herbicides: Agrochemicals can contaminate surface water, ground water and the atmosphere (Garibay *et al.*, 2001) leading to multiple problems in terms of both biodiversity losses, loss of ecosystem function and other problems for humans such as contamination of drinking water. There are also an increasing number of regulations being placed on herbicides and so by reducing their usage, farmers become less reliant on individual active ingredients which could be withdrawn. So, by aiming to minimise the amount of herbicide used on farms the benefits would be multiple: production costs would be reduced, the effective life of some active ingredients would be prolonged, environmental concerns would be addressed, and there would be less reliance on this singular method of control encouraging greater adoption of integrated weed management programs.

The decreasing number of chemical products available to farmers and the increasing pressures to reduce pesticide use puts a growing emphasis on the optimisation of current techniques and finding alternative approaches (Grundy, 2003). An increasing level of integrated weed management prevents reliance on one particular management option, such as herbicides. However, designing effective integrated weed management programs is a complex task and requires an in-depth understanding of the dynamics of weed populations (Fernandez-Quintilla, 1988) as many cultural control methods focussing on the species' biology and ecology are often incorporated into such programs. For example, delaying drilling of the crop can allow a greater level of germination prior to sowing. This cohort of weeds can then be removed with a single application of herbicide early in the season. However, this technique relies on a good understanding of the periodicity of emergence of different weed species. One option suggested for reducing the amount of herbicides used for weed management is through the consideration of economic thresholds, or particular densities of weeds below which there is little economic reason to spray herbicides as the cost of inputs will exceed yield losses. However, for *A. myosuroides* it is difficult to establish such damage thresholds for herbicide application, as there is great variability in the yield response (Moss, 1980).

Another option might be through the use of precision management techniques such as the spatially variable application of herbicides, or patch spraying.

The distributions of many weed populations are heterogeneous within individual fields; often showing aggregation at various densities, with patches of varying size and shape. No consistent patterns are observed across species (Cardina *et al.*, 1997; Dieleman *et al.*, 2000; Walter *et al.*, 2002; Heijting *et al.*, 2007). However, despite some level of unpredictability in patch size and location, this spatial heterogeneity within weed populations can be incorporated into population dynamics models (van Groenendael, 1988) allowing it to be studied in detail, and management regimes to be developed that incorporate the idea that weeds are spatially variable and so should be managed as such. Most crop management practices are aimed at minimizing heterogeneity to optimize yield (Pollnac *et al.*, 2008) and so it follows that site-specific management of weeds can improve crop yield through the minimisation of heterogeneity within the crop. *Alopecurus myosuroides*, like many weed species, grows in patches that vary in size and shape (Wilson & Brain, 1991; Krohmann *et al.*, 2006). This makes it an ideal candidate species for site-specific weed management.

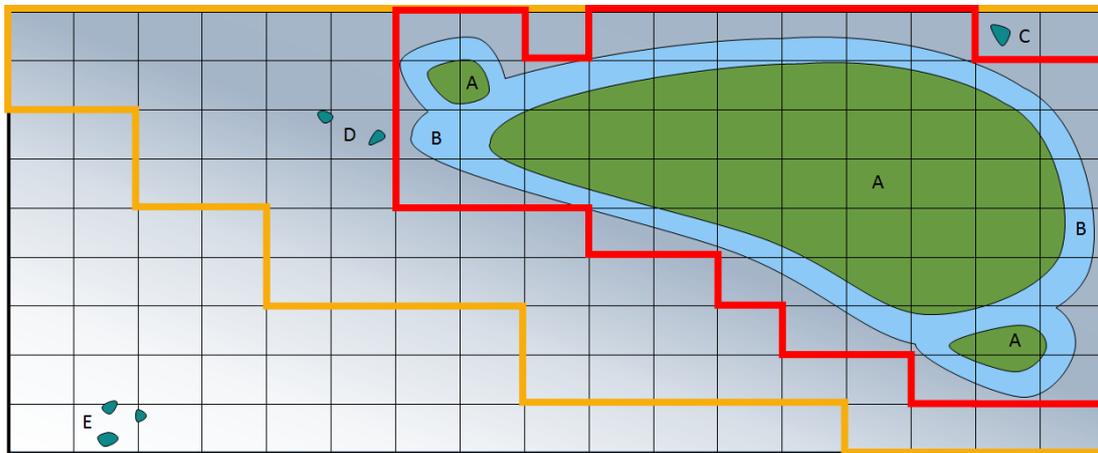
### 1.1.1 Site-Specific Weed Management

The intrinsic patchiness of weeds can lead to inefficiencies in their control, as often a farmer will base their decision to spray a field on the presence of weeds at any location within the field or on overall densities, whereas in reality there might be large areas of the field that require no spraying, causing the farmer to waste time, money, and chemical (Cardina *et al.*, 1997). However, advances in modern agronomy allow much greater precision, and as such it is now possible to take into account finer scale spatial variations than may have been achievable in the past. This is already commonplace in many aspects of farming. Information-based management systems to adapt fertiliser distribution across the field were first introduced in the mid-1980s (Gebbers & Adamchuk, 2010) and since then precision farming techniques including GPS steering, soil mapping, and variable rate seeding are becoming increasingly popular; with the proportion of UK farmers who implement these techniques increasing over recent years (Defra, 2013).

The concept of site-specific weed management, specifically patch spraying (see

Figure 1.3) is gathering interest. This takes into account the spatial variability of weeds either through intermittent spraying based on observed weed density at different locations or by modelling the thresholds for weed density above which it is economic to spray (Garibay *et al.*, 2001). This results in reduced chemical cost and more accurate application of control practices where required (Dieleman *et al.*, 2000). However, the economic benefits of site-specific weed management are related to both the proportion of the field that is infested as well as the number of weed patches. Therefore, to determine the economic viability of this approach and subsequently to implement any patch spraying program, the distribution of the weeds within the field must be mapped. Treatment maps can be created with the use of manually collected data on weed distributions, which is time-consuming and costly (Rew & Cousens, 2001), or through real-time detection of weeds using optical sensors. This real-time approach is still in development, and whilst already feasible is not yet at the stage of widespread commercialization (e.g. Murdoch *et al.*, 2010). A third approach, in development, that shows some potential for rapid map production is through remote sensing and multi-spectral imaging. However, the required knowledge to implement this is still lacking (Rew & Cousens, 2001). When any of these methods are implemented for *A. myosuroides*, the current practice is to map the distribution of seed heads in the summer as these are easily detectable, often growing above the crop.

Knowing the spatial distribution of weed species is vital when implementing precision management techniques and can be one of the barriers facing the uptake of this type of management due to the time-consuming or costly nature of map creation. However, site-specific management can be facilitated if weed patches are stable in location. Patch stability allows weed maps produced in one year to be used for site-specific control in future years (Pollnac *et al.*, 2008). This can be particularly useful when considering the application of pre-emergence herbicides as there is no visual indication of weed distributions at the time of their application and so it would be useful to use the known distribution of weeds from the previous year to help inform decision-making (Colbach *et al.*, 2000). The stability of *A. myosuroides* patches is not an area that has been extensively examined, but from the relatively few experiments that have studied patch stability it is apparent that patches can be fairly stable (Wilson & Brain, 1991) with core areas of *A. myosuroides* patches moving only 3–4 m over several years (Lutman *et al.*, 2002). This spatial stability does not, however, confer stability in weed density (Cardina *et al.*, 1997). Colbach *et al.*, (2000) demonstrated this effect through correct prediction



**Figure 1.3.** Diagrammatic representation of the principles of patch spraying. Patch spraying often involves the mapping of weed patches within fields (A), either through manual surveying of heads or real-time detection. A buffer zone (B) is then drawn around these mapped patches to allow for the spread of the patch in the following season. The field is then divided into grids of a manageable size — often the width of the spray boom — and all grid cells that contain the patch and buffer zones will be sprayed (cells within the red line). This approach does not account for individuals dispersing outside of the buffer zones (C), being dragged long distances by the cultivator (D) or entering the field from the margin (E). If a suite of soil properties could be identified that are favourable to *A. myosuroides* (grey areas). Then we may be able to identify “weed vulnerable zones” and spray accordingly (cells within the yellow line). This presents a more conservative approach as a greater area of the field is sprayed, making it more appealing to farmers, yet still reducing the overall use of pesticide. It is likely that in this instance the seeds that fell outside of the original buffer zones, but are captured within the weed vulnerable zone, would have gone on to form a new patch (C and D). However, the seeds entering the field from the margin to land outside of the weed vulnerable zone (E) would not present a risk.

of the location of patches from previous years' maps but the density at the site was often incorrectly estimated. They also showed that the greater the time between sampling and prediction the less accurate the prediction becomes. This means that whilst it may be possible to use maps from previous seasons as treatment maps they may be unsuitable in a threshold type approach.

### **Uptake of Site-Specific Weed Management**

Despite the numerous benefits of introducing patch spraying as a form of weed management, it is not being readily taken up as a standard management tool. There may be many reasons for this. First, with the growing problem of herbicide resistance on many farms, spraying is not always the best form of management and many cultural controls are now being used more commonly than in recent years. Also, resistance can lead to very large seed densities or large patches, which can make patch spraying less profitable (Audsley, 1993).

The cost and availability of equipment required for patch spraying can be a deterrent to the uptake of patch spraying. Equipment is required to recognize, quantify, and indicate spray actions, all of which can be expensive. Not all of the equipment is essential but without it, a lot of time and labour is required for sampling the field to obtain the data needed to construct maps used to direct the sprayer (Colbach *et al.*, 2000). Also, many of the technologies developed so far are dedicated to specific crops and ranges of weed species, which limits the range of usage (Christensen *et al.*, 2009). However, if a farmer is already using some precision management techniques such as mapping the yield through the combine and varying fertilizer on a spatial basis then they will already have a lot of the equipment required for patch spraying (Lutman *et al.*, 2002).

Finally, a change to patch spraying goes against current practice and often faces resistance from many farmers, despite the fact that an unwillingness to adapt treatments to spatial heterogeneity leads to inefficiencies in control measures (Colbach *et al.*, 2000). This unwillingness to implement site-specific weed management may also stem from the perceived risk of missing individuals that grow outside of currently established patches. Individuals may enter the field from elsewhere or a patch may expand due to increased dispersal from highly dense patches or through cultivation. If these individuals remain

unsprayed there is a risk they will turn into new patches outside of currently mapped zones (Figure 1.3). Failure to control *A. myosuroides* is known to lead to large levels of seed return (Moss, 1980) and so many farmers have an innate conservatism when it comes to the control of this pernicious weed and will often adopt a zero-tolerance approach. The incorporation of buffer zones into spray maps is a general measure taken to try and combat this, however this does not account for seed spreading outside of the immediate area surrounding the patch or entering the field from elsewhere.

### **Current Research into Site-Specific Weed Management**

In recent years, the idea of studying the spatial distribution of weeds with intent to introduce a site-specific aspect to their management has been an area that has had growing interest. The introduction of satellite spatial technology in the 1990s introduced the possibility of locating weed patches in the field (Lutman *et al.*, 2002) and this is something that is now being explored further with the use of unmanned aerial vehicles (e.g. Castaldi *et al.*, 2016, López-Granados *et al.*, 2016a, López-Granados *et al.*, 2016b, Pérez-Ortiz *et al.*, 2016). Work examining the possibility of real-time mapping of weeds (e.g. Murdoch *et al.*, 2010, Tian *et al.*, 2000) is also ongoing. However, both of these techniques rely on mapping current weed distributions, and so neither addresses the concern surrounding the risk of missing individuals that disperse outside of currently established patches. In this project I address these concerns by identifying areas of a field vulnerable to invasion by *A. myosuroides*. This would allow the creation of treatment maps without first mapping the distribution of the weed within the field.

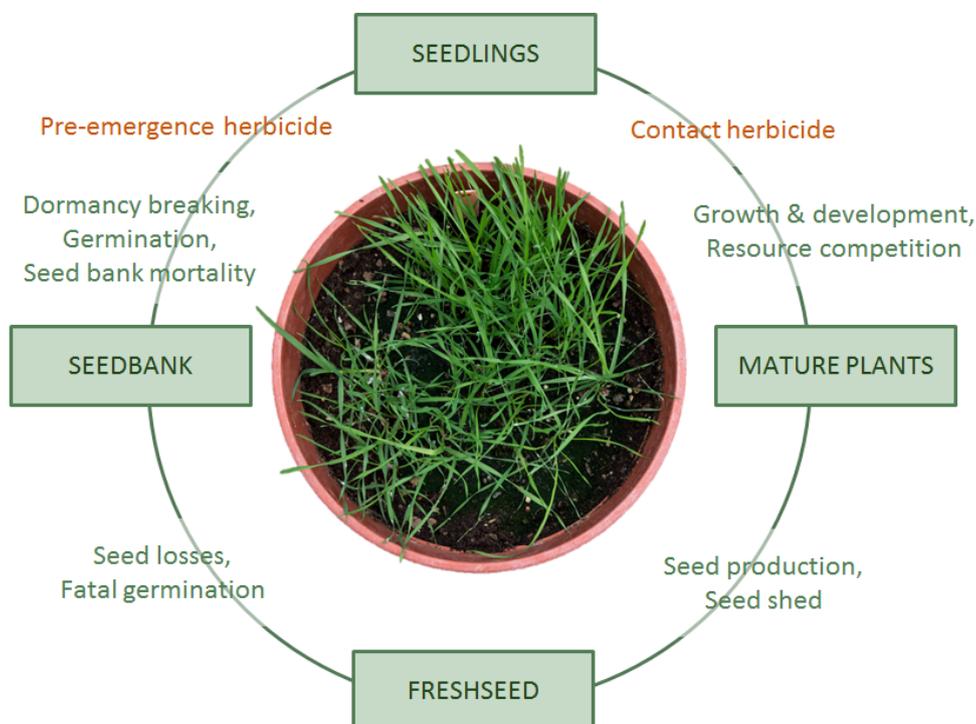
## **1.2 Within-Field Spatial Heterogeneity in Weed Distributions**

One possible option for site-specific weed management that addresses concerns about individuals establishing outside of mapped patches is to identify parts of the field that are vulnerable to invasion by a weed and are at risk to the establishment of a new patch. These “weed vulnerable zones”, once identified, could be used in the creation of spray maps to guide the precision application of herbicides (Figure 1.3). By defining all parts of the field that are vulnerable to weed invasion the concept of applying buffer zones to existing patches is incorporated, as well as capturing any individuals that may enter the

field from elsewhere. In order to be able to identify such weed vulnerable zones within a field it is important to understand what influences the observed spatial heterogeneity in the weed population. Weed patches can be modelled simply by using mathematical rules allowing for aggregation as random events (Audsley, 1993). In a uniformly infested field, this will give rise to a patchy population (Lutman *et al.*, 2002). However, it is likely that these random events are not the only factor causing patchiness in the population as the agroecosystem is a complex interaction of biological mechanisms, agricultural activities, and environmental variables.

### 1.2.1 Weed Biology and Ecology

Many aspects of the biology of weed species make them intrinsically prone to aggregation. By assessing the life-cycle of a given species the effects on patchiness can be considered (van Groenendael, 1988). The life-cycle of *A. myosuroides* is typical of an annual grass and comprises four main stages: the seedbank, seedlings, mature plants and fresh seed (Figure 1.4). Impacts on any of these stages, or processes occurring between them, has the potential to affect the distribution of the population and so may lead to patchiness within fields.



**Figure 1.4.** The life-cycle of *A. myosuroides*. Biological processes are shown in green and chemical interventions in orange.

One of the main causes of spatial heterogeneity is seed dispersal (van Groenendael, 1988). Seed dispersal range determines the possibility of new site colonisation (Maréchal *et al.*, 2012) and depends on the weed plant and seed characteristics as well as external factors such as wind speed for anemochorous species. For *A. myosuroides*, despite being primarily dispersed by barochory, increasing wind speed can increase the number of seeds dispersed, and the distance that they are dispersed (Colbach & Sache, 2001). For most species with these dispersal types natural seed dispersal only occurs over short distances, causing many new plants to develop in a small area around the parent plant. This can form the start of a patch. Distribution patterns are often more dense along the edge of a field suggesting border effects, as seeds will only disperse short distances from parent plants located in hedgerows or headlands (Cardina *et al.*, 1997). As seedlings mature, and increase in size, density dependent effects will begin to become important in determining survivorship and seed production (Dieleman *et al.*, 2000), as such patches can become self-regulating with plant densities levelling off after several years (Moss, 1990).

As well as the intrinsic biology of the weed itself other ecological factors within the community can also play an important role in controlling the spatial distribution of weed species. For example, competition with the crop and other weed species, mediated by the local environment, can affect the distribution of a weed (Radosevich *et al.*, 2007). Herbivory and disease can also be important in regulating population size and distribution.

In terms of improving weed control, the biology of the weed presents some opportunities for exploitation. If we know about typical dispersal ranges for a given species, then this can be incorporated into current models for patch spraying through the addition of buffer zones around mapped patches to encompass all areas where the weed might typically be able to disperse (Rew & Cousens, 2001). If these buffer zones are omitted then these patch boundaries could act as the foci for the spread of new patches (Paice *et al.*, 1998). Modern high-yielding varieties often demonstrate less tolerance to competition from weeds (Oerke, 2006) and so the typical competitive ability of a given weed species can be exploited by choosing a crop cultivar that is more competitive against that weed species (Andrew *et al.*, 2015).

### 1.2.2 Agronomy

Agronomic factors can also influence the spatial distribution of weed species with the agronomic history of the field having a large influence on weed distribution. For example, former field boundaries may have a higher density of weed seeds than the rest of the field due to the bigger seed bank from old hedgerows (Lutman *et al.*, 2002). Historic fertility patterns could also affect weed growth and their competitive ability, as well as that of the crop, in much the same way as current nutrient management does (Dieleman *et al.*, 2000).

Variability in herbicide application across the field due to drift can influence patch formation as areas receiving less or no herbicide are likely to lead to the persistence of weeds, which would otherwise have been controlled (Williams II *et al.*, 2001). This leads to commonly observed increases in weed densities at the edges of fields. However, organic systems also display non-random patterns of weed distribution (Pollnac *et al.*, 2008) indicating that herbicide control failure is not the only intervening factor. Poor crop establishment in parts of a field may lead to the development of a patch, where competition is reduced (Lutman *et al.*, 2002). Often, when a patch forms due to control failure, there will be a large seed return in following years leading to patch longevity (Lutman *et al.*, 2002).

Dispersal of seed due to cultivations can also be important in determining where weed seeds are distributed. In many systems, there has been shown to be a directional effect with weeds forming elliptical patches of longest dimension in the direction of the crop rows (Colbach *et al.*, 2000). This is thought to be due to the movement of seeds by agricultural tillage and harvesting machinery. Large awned seeds are more likely to be spread in this manner as they can become easily trapped in the machinery (Lutman *et al.*, 2002) with particularly large seeds such as wild oat being moved up to 30 m by equipment such as combine harvesters (Lutman *et al.*, 2002). There is also the possibility of mature plants getting caught on farmland machinery and seeds being dispersed long distances (Pollnac *et al.*, 2008) allowing the formation of new patches (Lutman *et al.*, 2002). Dispersal of seeds in the direction of crop rows does not always occur through human intervention. It can also occur due to natural seed dispersal in tall crops where the weed seeds can move more freely in the rows between crops compared to their ability to move across the crop rows (Colbach *et al.*, 2000). In shorter crops,

where the weed flowers are above the crop canopy, this type of natural seed dispersal is more likely to be uniform (Paice *et al.*, 1998).

Cultivation can also contribute to the vertical movement of weed seeds in the soil profile (Moss, 1990). This can be exploited by farmers by choosing only to use deep cultivations infrequently. These type of cultivations bury large numbers of seed at depth. In the intervening years shallow cultivations will not return these seeds to the surface and so viability levels will decrease whilst the seeds remain at a depth from which they cannot germinate. Another opportunity that these agronomic effects on patch distribution presents for improved weed management is to clean machinery before moving between farms in order to reduce the spread of weeds. This can be particularly important in reducing the introduction of seed to new locations.

### 1.2.3 Environment

In addition to the biology and ecology of weeds, and agronomic factors; the environment is a large determinant in the location of weed patches and this is the main focus of this project. Many aspects of the natural environment vary spatially, and it is known that the distribution of weeds can be strongly affected by abiotic factors including light, precipitation, temperature, soil type, pH and moisture (Radosevich *et al.*, 2007). It is therefore important to consider the spatial distribution of these abiotic factors when considering causes of patchiness in weed populations. However, covariation of site properties and weed distributions is not something that is well understood (Dieleman *et al.*, 2000). Abiotic and biotic factors are strongly related and so a plant's response to them is hard to separate out (Radosevich *et al.*, 2007). For example, the density of the plant canopy can have a strong effect on the quality and quantity of radiation received by other plants in the understory (Radosevich *et al.*, 2007). In many instances several environmental variables may be linked and show correlations between them, making it difficult to disassociate one from another when trying to determine the cause of spatial aggregation in weed population. For example, local topographic variations may cause variation in weed distribution but this may be linked to multiple soil factors, for example soil moisture and temperature (Lutman *et al.*, 2002).

Abiotic factors can be an important determinant in whether a site is favourable for growth, as if a seed lands in an environment unsuitable for its germination it is

unlikely to germinate, or to compete successfully. Therefore spatial heterogeneity of weed populations is considered to be partially determined by the local distribution of sites with suitable abiotic conditions (van Groenendael, 1988). Vertical variation in soil can also result in variable seed survival, dormancy, and therefore emergence (Cardina *et al.*, 1997). There is also a substantial environmental influence on seed dormancy (Finch-Savage & Leubner-Metzger, 2006). Natural seed burial in a minimum or no tillage system is also dependent on soil texture with slower seed burial in clay soil than in soil of coarser texture (Benvenuti, 2007). However, this natural seed burial is dependent on seed weight and so may only lead to sufficient depth of burial to prevent germination in some weed species. The distribution of some species can be affected by soil type. For example, *Galium aparine* L. (cleavers) and *A. myosuroides* are often associated with soil of larger clay content, whereas other species such as *Senecio vulgaris* L. (groundsel) prefer lighter soil (Lutman *et al.*, 2002). Other soil variables such as carbon, water, and macronutrients have been shown to be correlated to weed distributions (Lutman *et al.*, 2002) and are rarely homogeneously distributed in the soil (Robertson & Gross, 1994). The influence of various soil factors on weed abundance can often be related back to their effect on soil moisture and water holding capacity (Dieleman *et al.*, 2000). Availability of water in the soil is important in many aspects of the weeds' life-cycle, particularly in the early growing season (Dieleman *et al.*, 2000).

Soil properties not only affect the distribution of weeds directly but they can also have an indirect effect in terms of altering the efficacy of some herbicides (Lutman *et al.*, 2002). High amounts of clay and organic carbon in soil can lead to the sorption of most herbicides (Gaston *et al.*, 2001) and the pH of the soil can also affect the sorption of ionizable herbicides as well as several chemical degradation mechanisms (Gaston *et al.*, 2001). Sorption of herbicides will reduce the amount of herbicide taken up by the plant and through this mechanism, different soil types will affect the level of control achieved through herbicide use. If this differs spatially across the field, then it may lead to differential control across the field and lead to the establishment of weed patches where herbicide control is reduced.

Weeds can improve soil quality and fertility in a way that is not achieved by crop plants alone, as they help reduce soil erosion; slowing down the rate of nutrient loss (Ziska & Dukes 2011). Weeds also contribute to nitrogen cycling in agroecosystems (Patriquin, 1986) as well as helping to accumulate other nutrients within the system

(Swamy & Ramakrishnan, 1988) and so it is possible that through being aggregated the weeds ameliorate the system allowing longevity of the patch by making conditions more favourable for germination of new individuals.

The effect of soil properties on the patchiness of weed populations presents an opportunity for site-specific weed management as the environments that are favourable for weed growth are much more likely to remain stable in location than a weed patch might and so if these areas can be targeted, rather than the patch itself, then the risks of missing individuals dispersing outside of already established patches or entering the field from elsewhere could be minimised.

### 1.3 Objectives

*Alopecurus myosuroides* has known associations with some soil types. It has traditionally been found in poorly drained, heavy textured soil and is described by farmers as a marsh weed. However, changing cropping practices and the reduction in control because of evolved herbicide resistance may have allowed it to expand its range into lighter soil (Holm *et al.*, 1997). In addition to these coarse-scale associations with certain soil types, there is some evidence that the within-field distribution of *A. myosuroides* is also associated with variation in soil properties (Radosevich *et al.*, 2007; Holm *et al.*, 1997; Lutman *et al.*, 2002; Dunker & Nordmeyer, 2000). The principle of the ecological niche dictates that a plant will grow in the environment most favourable to it and so we can assume that there is some sort of environmental variation allowing it to grow better in certain areas of the field than others. Our lack of detailed understanding of the ecological niche of this important economic pest is currently preventing the implementation of patch spraying based on that knowledge. If we can understand what drives the within-field distribution of this species, we would be better equipped to manage this species in a more sustainable manner through site-specific weed management. We could also reduce the risks associated with current methods, where individuals growing outside of established patches could be missed, by identifying weed vulnerable zones within fields (Figure 1.3).

**My main objective is to identify environmental determinants of *A. myosuroides* patch location and use these to define weed vulnerable zones.** In order to meet this

main objective, I will combine field work, pot experiments and modelling to test the following hypotheses reported in Chapters 3–6 respectively (Chapter 2 presents a new sampling methodology to address Hypothesis 1):

### 1.3.1 Hypotheses

**Hypothesis 1: The within-field spatial distribution of *A. myosuroides* is associated with the spatial distribution of environmental variables at scales appropriate for management.**

Previous studies that have attempted to investigate the link between *A. myosuroides* patch locations and soil properties have been limited in their scope; only sampling at a single scale (e.g. Dunker & Nordmeyer, 1999 and 2000; Lutman *et al.*, 2002). This has led to discrepancies in conclusions, with conflicting results being obtained from different studies. I resolved these discrepancies by examining the scale-dependence of correlations between the distribution of *A. myosuroides* and various soil properties through the use of a novel nested sampling design (Chapter 2). I investigated if any observed relationships were consistent across fields and at what scale the strongest relations were observed (Chapter 3) to determine if these were appropriate for management. I also identified which environmental properties provided the most useful prediction of within-field *A. myosuroides* distributions (Chapter 3).

By testing this hypothesis I improved our understanding of the habitat niche of this important agricultural weed and therefore our understanding of the environmental influencers on its within-field distribution. This contributed to my main objective by identifying the soil properties that correspond most with the within-field distribution of *A. myosuroides*, and that should be considered when locating weed vulnerable zones within fields.

**Hypothesis 2: Soil organic matter, moisture, and pH affect the life-cycle of *A. myosuroides* from germination to seed return.**

The abiotic environment exerts many influences on plants. Temperature and moisture are particularly important for germination (Forcella *et al.*, 2000) and this is well

characterised for *A. myosuroides* (Colbach *et al.*, 2002a and b). However, the influence of other environmental properties, particularly relating to the soil, on germination and the rest of the life-cycle, are less well understood.

Through a series of pot experiments I investigated the effect of soil organic matter, moisture, and pH on all aspects of the life-cycle of *A. myosuroides* from germination to seed return (Chapter 4). I chose to investigate these soil properties as they were found to be particularly important in the testing of Hypothesis 1 (Chapter 3).

By testing this hypothesis, I increased our understanding of how these soil properties affect the growth and competitive ability of *A. myosuroides*. This enabled me to better understand the role of variation in the soil in determining the within-field distribution of this species and so, in part, to determine the causality of the relationship between the spatial distribution of soil properties in fields and the within-field distribution of *A. myosuroides*.

**Hypothesis 3: Soil organic matter affects the efficacy of flufenacet and pendimethalin against *A. myosuroides* and the ability of the weed to withstand sub-lethal doses of those herbicides.**

Organic matter in the soil can lead to adsorption of herbicide (Farenhorst, 2006). Different herbicides may be more or less adsorbed by organic matter, dependent on their physical and chemical properties (Nordmeyer, 2015). As pre-emergence herbicides are applied directly to the soil, it is particularly important to understand how varying soil properties within fields may be affecting their efficacy. I investigated the effect of soil organic matter on the efficacy of two commonly used pre-emergence herbicides for *A. myosuroides* control, and whether the amount of soil organic matter plays a role in the resulting sub-lethal effects (Chapter 5).

By testing this hypothesis I was able to determine whether the effect of soil on *A. myosuroides* was only through direct effects on the weed itself or whether there are also indirect effects on its distribution, through a modification of management practices; in this case pre-emergence herbicides. This contributes to my main objective by determining how current management practices may be contributing to *A. myosuroides* patch locations and if this needs to be considered in addition to the current distribution of the weed when identifying weed vulnerable zones.

**Hypothesis 4: The scale-dependent relationships between soil properties and the density of *A. myosuroides* observed in fields is an emergent property of the effect of the soil on the various aspects of the weed's life-cycle.**

Building on the modelling work of Moss (1990), Paice *et al.* (1998), and Colbach *et al.* (2006), I developed a life-cycle model for *A. myosuroides* that incorporates natural dispersal of the weed seeds as well as their dispersal by cultivation (Chapter 6). Based on the results of my investigations in Chapters 4 and 5, I developed functions to describe the effect of soil on various aspects of the life-cycle of *A. myosuroides* and included these in the model. I verified the ability of the model to replicate the field results obtained in Chapter 3 by replicating the sampling regime (Chapter 2) in the resulting fields and seeing if the scale-dependent relationships observed in the field were an emergent property of the modelling process (Chapter 6).

The development of this model allowed me to pull together all previous strands of this project to investigate whether modelling the changes to each aspect of the *A. myosuroides* life-cycle caused by different soil properties in a spatially heterogeneous environment could explain the within-field distributions observed on farms. By testing this hypothesis I could determine the possibility of identifying weed vulnerable zones within fields based on pre-existing or supplemented soil maps.

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## Chapter 2

# Designing a Sampling Scheme to Reveal Correlations Between Weeds and Soil Properties at Multiple Spatial Scales

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My main objective in this thesis is to identify environmental determinants of *A. myosuroides* patch location and use these to identify weed vulnerable zones. The first part of this objective — identifying environmental determinants of *A. myosuroides* patch location — has been previously considered (e.g. Dunker & Nordmeyer, 1999 and 2000; Lutman *et al.*, 2002). However, these studies were limited in their scope because they only sampled at a single scale. This led to discrepancies in their conclusions, with conflicting results being obtained from different studies, possibly due to their failure to account for scale. My first hypothesis addresses this by considering the scale-dependence of correlations between the distribution of *A. myosuroides* and soil properties. I sampled *A. myosuroides* density and soil properties across five fields according to an unbalanced

nested sampling design. This design allowed me to partition the correlation between the two variables of interest — *A. myosuroides* and each environmental variable — across spatial scales. In this chapter, I describe the nested design and method of analysis using one field as a case study. In Chapter 3, I present the results from all five fields.

The following was published in *Weed Research* **56** (1) 1–13 in February 2016. It outlines the process by which we designed the sampling scheme for use in the field trials detailed in Chapter 3, beginning with a design assuming equal variance at all scales of interest. Following the analysis of the data obtained, indicating that variance is not equal at all scales, we detail the optimization of the design, for use in further fields focussing sampling effort on the scales of most interest.

## 2.1 Summary

Weeds tend to aggregate in patches within fields and there is evidence that this is partly owing to variation in soil properties. Because the processes driving soil heterogeneity operate at various scales, the strength of the relations between soil properties and weed density would also be expected to be scale-dependent. Quantifying these effects of scale on weed patch dynamics is essential to guide the design of discrete sampling protocols for mapping weed distribution. We have developed a general method that uses novel within-field nested sampling and residual maximum likelihood (REML) estimation to explore scale-dependent relations between weeds and soil properties. We have validated the method using a case study of *A. myosuroides* in winter wheat. Using REML, we partitioned the variance and covariance into scale-specific components and estimated the correlations between the weed counts and soil properties at each scale. We used variograms to quantify the spatial structure in the data and to map variables by kriging. Our methodology successfully captured the effect of scale on a number of edaphic drivers of weed patchiness. The overall Pearson correlations between *A. myosuroides* and soil organic matter and clay content were weak and masked the stronger correlations at >50 m. Knowing how the variance was partitioned across the spatial scales we optimized the sampling design to focus sampling effort at those scales that contributed most to the total variance. The methods have the potential to guide patch spraying of weeds by identifying areas of the field that are vulnerable to weed establishment.

## 2.2 Introduction

Many weed species have patchy distributions in arable fields that can be strongly affected by their environments, in particular the soil (Radosevich *et al.*, 2007). The spatial variation of soil results from numerous processes operating at several spatial scales, and so the variation in some soil properties can also be patchy though not necessarily on the same scales as the weeds. As a consequence the relations between the abundances of weeds and particular soil properties can change from one spatial scale to another. This means that relations between the two variables found at the one scale might not hold at another (Corstanje *et al.*, 2007). In these circumstances, a small absolute correlation coefficient between a weed count and a soil property calculated from a simple random sample over a whole field, though statistically sound, could obscure strong relations at particular scales and be misleading.

Several investigators (e.g. Gaston *et al.*, 2001; Walter *et al.*, 2002; Nordmeyer & Häusler, 2004) have used grids for studying spatial variation in weeds. They have assumed some prior knowledge of the spatial scales of variation in the field, and that has led them to choose grid intervals that would capture the necessary spatial detail; they would not have wished to risk missing such detail by having too coarse a grid. However, sampling at fine scales would make sampling the whole of a large field very expensive and, almost certainly, unnecessarily so if the aim is to understand the general position of patches within the field rather than small changes in the location of patches. These difficulties associated with the design of discrete sampling protocols for studying weed patches, either as a tool for understanding weed ecology or mapping weeds to guide patch spraying, have been thoroughly reviewed by Rew & Cousens (2001). They highlighted the need to develop new analytical techniques to capture the effects of scale on the dynamics of weed patches and to optimize sampling. Partly because of the risk of discrete sampling at too coarse a resolution, they argued that ground-based continuous sampling was more appropriate for practical site-specific weed management applications. Whilst many mapping procedures can be done early in the season and used for control in the current season, real-time detection and control is difficult. For many grass weeds the current systems can only definitively identify the species of grass once it is flowering. This will be too late for the application of selective herbicides (Murdoch *et al.*, 2010). It is therefore also necessary to consider the risk of seedlings establishing outside the mapped patch when planning site-specific herbicide sprays in the following

season. An understanding of the edaphic drivers of weed patch dynamics and the scales at which they operate is both of theoretical interest to weed ecologists, and could allow these “weed vulnerable zones” to be identified based on maps of soil properties. Here we address these issues by applying sampling methodologies designed in the field of soil science to optimize sampling effort to the study of weed patches and how they may relate to environmental properties at multiple spatial scales.

We used the model system of *Alopecurus myosuroides* Huds. (black-grass) in winter wheat (*Triticum aestivum* L.) to demonstrate the potential of these methods. The distribution of *A. myosuroides* is patchy, and its density seems to depend to some degree on the nature of the soil (Holm *et al.*, 1997; Lutman *et al.*, 2002). We assumed no prior knowledge of the spatial scale(s) on which the weed varied in particular fields and so we explored its distribution in one particular field by sampling with a nested design followed by a hierarchical statistical analysis to partition the variance and covariances with soil properties according to spatial scale. In principle, nested sampling schemes allow the estimation of the components of variance for a variable across a wide range of spatial scales and to quantify the covariation and correlation between variables over that range. As we did not know beforehand what sizes of patches to expect or whether to expect variation and causal relations with the soil at more than one spatial scale, we designed a nested sampling scheme with a wide range of sampling intervals that we hoped would reveal the spatial scale(s) of variation in the weed and of its covariation with the soil. We used the method proposed by Lark (2011) to optimize our sampling scheme. The aim of the optimization was to partition the sampling across the scales so that the estimation errors for the components of variance were as small as possible with the resources available.

Our primary objective was to develop and validate a generic method to examine the relations between weed distributions and environmental properties at multiple spatial scales. We wanted to demonstrate a way of identifying the relevant scale at which the processes affecting weed patch dynamics operate. This could be a precursor to the use of data on environmental heterogeneity to support patch spraying or to guide the design of optimal sampling strategies for studying weed spatial dynamics. The case study reported here demonstrates the use of this methodology in one field and provides evidence to support the hypothesis that relations between soil variables and weed patches are scale-dependent.

## 2.3 Materials and Methods

### 2.3.1 Study Site

The field we chose for study is on a commercial farm in Harpenden, Hertfordshire, UK. It has long been in arable cultivation and is infested with *A. myosuroides*. It comprises two former fields from which the old boundary was removed some decades ago. The southern part of the field is generally flat, whilst the northern part slopes gently downwards towards the north. The soil is stony clay loam containing numerous flints and overlies the Clay-with-Flints formation. The soil grades from Batcombe series in the southern part to the somewhat more clay-rich Winchester series on the northern slope (Hodge *et al.*, 1984).

### 2.3.2 Sampling Scheme

To consider how the *A. myosuroides* patches vary in space and how that variation relates to soil properties at multiple spatial scales we examined the spatial components of variance and covariance. This allows us to express the patchiness of the weed's distribution in the field statistically. Estimates of the components of variance can describe the infestation at several scales, and from them one should be able to design better targeted sampling schemes for future surveys.

Youden & Mehlich (1937) first proposed a nested sampling design to discover the spatial scales of variation in soil. They sampled the soil at locations that were organized hierarchically into clusters separated by fixed distances. The nested sampling design had several main stations separated across the region. These correspond to the top level of the design (level 1). Within each main station they selected two substations (level 2) which were separated by a fixed distance (305 m) but with the vector joining the substations oriented on a random bearing. Within each substation at level 2 they selected a further two substations at level 3, this time separated by 30.5 m. The final level of replication within their design, level 4, was with pairs of substations within each level-3 substation, separated by 3.05 m. Soil samples were collected at each of the eight level-4 substations within each main station. An analysis of variance allowed them to partition the variance of each measured soil property into components associated with each level of the nested design.

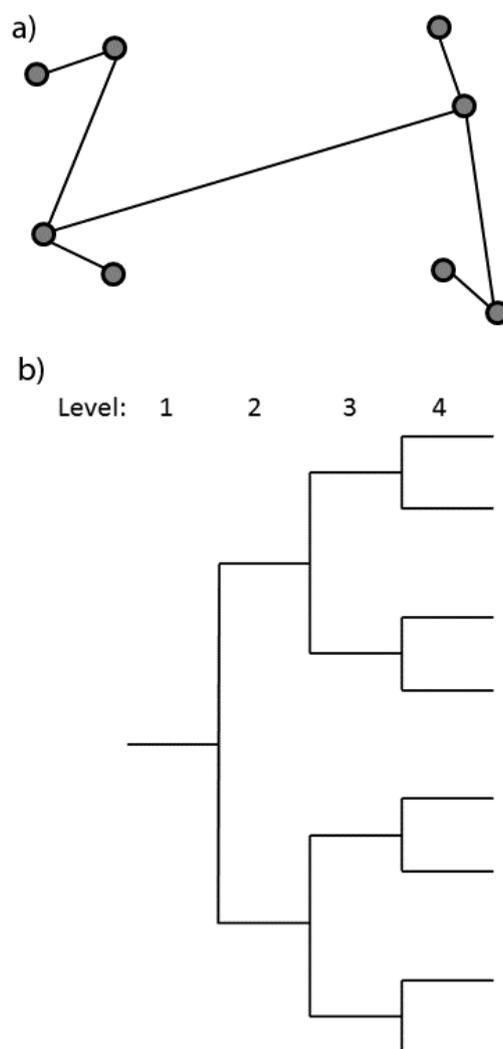
This nested design used by Youden & Mehlich (1937) is said to be balanced because any two substations at a given level have identical replication within them at lower levels of the design (Figure 2.1 b). Such designs become prohibitively expensive for more than a few levels, as the number of sample points doubles for every additional level of the design. Furthermore, there are many more fine-scale comparisons than ones at the coarser scales (Figure 2.1 a), and this is not necessarily an efficient distribution of sampling effort. For example, in the design shown in Figure 2.1 there are four pairs of points separated at the finest scale (level 4), whereas there are only two groups of points separated at level 3 and only one pair of groups of points separated at the coarsest scale within the design, level 2.

Several attempts have been made to economize on nested sampling without seriously sacrificing precision (see Webster *et al.*, 2006). Lark (2011) brought together the various strands of that research and proposed designs that are optimal compromises in the sense that they maximize the precision across all levels for given effort, based on the assumption that there is prior knowledge as to how the variation is partitioned across the levels. Here, we apply this approach, for the first time, to the study of weed patches.

The aim of the analysis of a nested sampling design is to estimate components of variance, or covariance, for the sampled variables that correspond to each scale of the hierarchy. As a basis for our study we adopted the following model:

$$\begin{aligned} \mathbf{Z}^u &= \mathbf{x}\tau^u + \sum_{i=1}^k \mathbf{M}_i\eta_i^u, \\ \mathbf{Z}^v &= \mathbf{x}\tau^v + \sum_{i=1}^k \mathbf{M}_i\eta_i^v, \end{aligned} \quad (2.1)$$

where  $\mathbf{Z}^u$  comprises  $n$  random variables by which we model our  $n$  observations of variable  $u$  (which is an index, not a power), and similarly for variable  $v$ , and  $k$  is the number of random effects in the model. In our case variable  $u$  is weed counts, and  $v$  is a measured soil property. One may develop this model for any number of variables. The term  $\mathbf{x}\tau^u$  equates to a vector of mean values for variable  $u$ . In our case the mean is constant for any one variable and so comprises the design matrix  $\mathbf{x}$ , which is an  $n \times 1$  vector of 1s, and  $\tau^u$  is the mean for variable  $u$ . The same applies for variable  $v$ . The terms in the summation on the right-hand sides are random effects in the model. There are  $k$  of these for each variable, each corresponding to one level of the nested



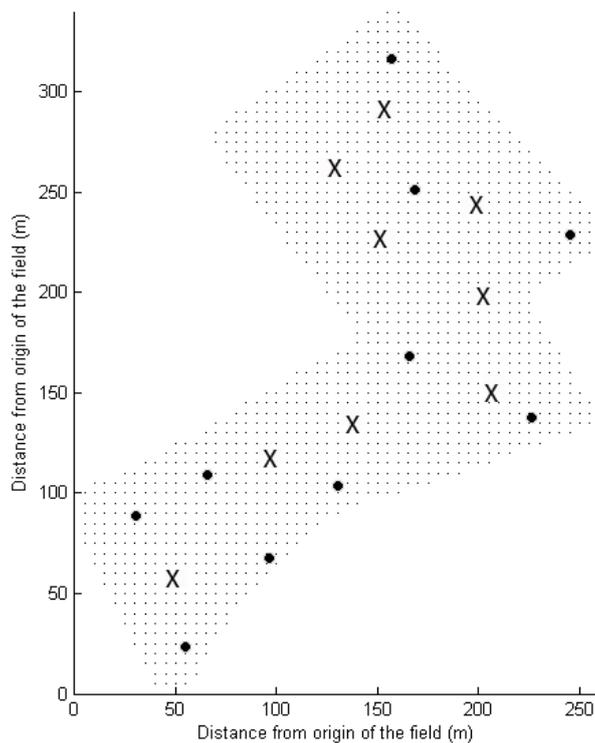
**Figure 2.1.** An example of a balanced nested sampling design; (a) the design as it might appear on the ground with circles indicating sampling points, (b) the topological tree from which the design is taken. The design is balanced in that there is equal replication at each level below the first.

sampling scheme, so  $k = 4$  in the case shown in Figure 2.1. The matrix  $\mathbf{M}_i$  is a  $n \times n_i$  design matrix for the  $i$ th level of the nested scheme; where  $n_i$  is the number of sampling stations at the  $i$ th level across the whole design. If the  $m$ th sample location belongs to the  $m_i$ th substation in the  $i$ th level of the design then  $\mathbf{M}_i[m, m_i] = 1$  and all other elements in the  $m$ th row are zero. The term  $\eta_i^u$  is a  $n_i \times 1$  random vector. The mean of its elements is zero and their variance is  $\sigma_{u,i}^2$ . This is the variance component for variable  $u$  associated with the  $i$ th scale. Similarly the elements of  $\eta_i^v$  have mean zero and variance  $\sigma_{v,i}^2$ . This extension of the nested spatial sampling scheme was proposed by Lark (2005) and has been used since in soil science (e.g. Corstanje *et al.*, 2007).

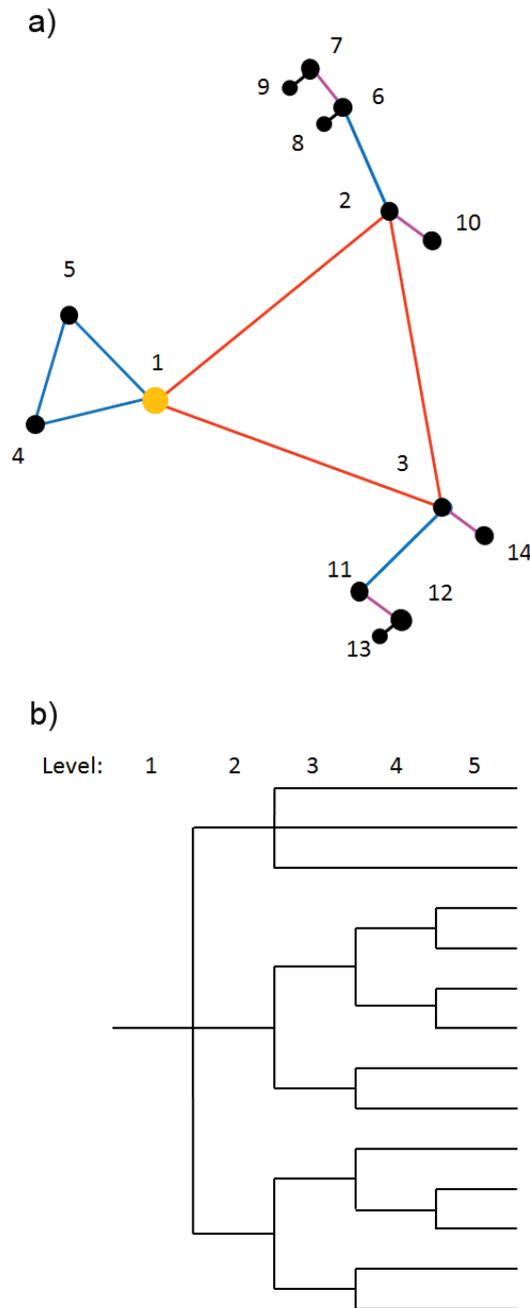
One novel aspect of our study was that at the outset we did not know the spatial scale(s) on which *A. myosuroides* varied nor whether the variances differed substantially from scale to scale. We therefore assumed the variances to be equal at all scales, and designed a sampling scheme accordingly. Our design is as follows with five levels in the hierarchy.

Nine main stations were spaced approximately 50 m apart across the field (Figure 2.2); this corresponds with level 1 of the hierarchy. Sampling sites were nested in groups at each main station (Figure 2.3 a). The distances between sites at level 2 in the design were 20.0 m, at level 3 the sites were spaced 7.3 m apart, those at level 4 were 2.7 m apart, and those at level 5 were spaced 1.0 m apart. The distances were fixed, but the directional bearings were randomized independently to satisfy the requirements of the model (Equation 2.1). Figure 2.3 b shows the structure as a topological tree, which is evidently unbalanced in that the replication is not equal in all branches of the tree. To improve our maps of *A. myosuroides* distribution and associated soil properties we added ten more sampling points, to give a total of 136 sampling points across the field. These additional points were added to fill the larger gaps in the coverage and thereby enable us to diminish the errors in maps made by kriging (Figure 2.2).

The positions for the main stations at the 1st level of the design were located in the field by GPS with subsidiary points located by their distance and orientation from the main station by tape measure and compass. Square quadrats (0.5 m<sup>2</sup>) were placed on the ground with their south-west vertices at the sampling point. All locations were subsequently geo-referenced with an RTK GPS (Topcon Positioning Systems, Inc., 7400 National Drive, Livermore, CA USA 94550) with a quoted resolution of 5 cm.



**Figure 2.2.** Location of sampling points within the field in Harpenden. The field is marked by grey dots. The locations of the nine main stations are shown as crosses. The ten extra sampling points are shown as closed discs.



**Figure 2.3.** Nested sampling design used in the field in Harpenden. (a) The design as one instance might appear on the ground with vertices labelled as the numbers 1–14. The yellow disc indicates the main station of the motif. Red lines represent nodes spaced 20 m apart, blue lines indicate 7.3 m, purple lines link points 2.7 m apart and black lines link those 1 m apart. (b) Topological tree of nested sampling design used in the field in Harpenden. The design is unbalanced as replication is not equal at all branches of the tree.

*Alopecurus myosuroides* individuals within each quadrat were counted in late October 2013 while the plants were at the one- to two-leaf stage. No pre-emergence herbicide had been used on the field.

### 2.3.3 Soil Analyses

Two cores of soil were taken from each quadrat with a half-cylindrical auger of diameter 3 cm to a depth of 28 cm on 21 January 2014 while the soil was at field capacity. The depth at which the clay layer was first visible was noted in each of the two augers to indicate the depth of cultivation. If the clay layer was not reached within the 28 cm then a value of 30 cm was assigned. The average of the two replicates was then recorded. The gravimetric water content was measured in layers 0–10 cm and 10–28 cm by loss on oven-drying at 105°C. Other variables were measured on samples pooled from the two cores within each quadrat. Organic matter was measured by loss on ignition. Available phosphorus (P) was measured in a sodium bicarbonate extract at pH 8.2. The pH was measured in water, and soil texture (particle-size distribution) was determined by laser diffraction. Stone content by both volume and mass was measured on a core of 76 mm diameter taken to depth 97 mm from the south west outside corner of each quadrat.

### 2.3.4 Statistical Analyses

A balanced design would lead to a straight forward analysis of variance (ANOVA) from which the components of variance are readily estimated. Analysing data from an unbalanced design is more complex. Gower (1962) provided formulae for computing the components from an ANOVA. The method now favoured on theoretical grounds is the residual maximum likelihood (REML) estimator due to Patterson & Thompson (1971) and is the one we used. Within the REML model (Equation 2.1), the terms  $\eta_i^u$ ,  $i = 1, 2, \dots, k$  and  $\eta_i^v$ ,  $i = 1, 2, \dots, k$  are the random effects. The assumption is that the concatenated  $2n \times 1$  random vector  $\left[ [\mathbf{Z}^u]^T [\mathbf{Z}^v]^T \right]^T$  has a joint multivariate normal distribution with  $2n \times 2n$  covariance matrix:

$$\mathbf{V} = \sum_{i=1}^k \begin{bmatrix} \sigma_{u,i}^2 \mathbf{M}_i \mathbf{M}_i^T & C_i^{u,v} \mathbf{M}_i \mathbf{M}_i^T \\ C_i^{u,v} \mathbf{M}_i \mathbf{M}_i^T & \sigma_{v,i}^2 \mathbf{M}_i \mathbf{M}_i^T \end{bmatrix} \quad (2.2)$$

where the superscript T denotes the transpose of a matrix. The variance and covariance components for each scale are the random effects parameters which are estimated by REML. We calculated Pearson correlation coefficients for all data to show correlations when scale is ignored. Note, however, that this does not give an unbiased estimate of the correlation because it ignores the dependency structure imposed by the sampling and is therefore a somewhat arbitrarily weighted combination of the correlations at different scales. Following partitioning of the components of variance at the different spatial scales, estimates of the correlations ( $\hat{\rho}$ ) at each scale ( $i$ ) between *A. myosuroides* and the soil properties were calculated by

$$\hat{\rho}_i^{u,v} = \frac{\hat{C}_i^{u,v}}{\hat{\sigma}_{u,i}\hat{\sigma}_{u,i}} \quad (2.3)$$

where the variables  $u$  and  $v$  are *A. myosuroides* counts and the soil property, respectively, and the terms with the hats are the REML estimates of their covariances ( $C$ ) and standard deviations ( $\sigma$ ). Where the estimated components of variance given by REML were non-positive no associated correlation coefficient was calculated. Confidence intervals for the correlations were calculated by Fisher's  $z$ -transform, with degrees of freedom appropriate to the number of sampled pairs at the corresponding level of the design.

Variograms were estimated and modelled from all data points from both the sampling design and the ten additional points to quantify the spatial structure in the variance of the measured variables. We did this using GenStat (Payne, 2013). Semivariances were calculated by the method of moments (Webster & Oliver, 2007):

$$\hat{\gamma}(\mathbf{h}) = \frac{1}{2m(\mathbf{h})} \sum_{j=1}^{m(\mathbf{h})} \{z(\mathbf{x}_j) - z(\mathbf{x}_j + \mathbf{h})\}^2 \quad (2.4)$$

where  $z(\mathbf{x}_j)$  and  $z(\mathbf{x}_j + \mathbf{h})$  are the observed values at two locations separated by lag  $\mathbf{h}$ , and  $m(\mathbf{h})$  is the number of pairs of points at that lag. By incrementing  $\mathbf{h}$  we obtained an ordered set of values to give the experimental variogram, which is a function of the expected mean squared difference between two random variables,  $z(\mathbf{x})$  and  $z(\mathbf{x} + \mathbf{h})$  at locations  $\mathbf{x}$  and  $\mathbf{x}_j + \mathbf{h}$ . The variation appeared to be isotropic and so we treated the lag as a scalar in distance only.

In the case of *A. myosuroides* counts, where the distribution was skewed, a log

transformation was used before estimation of the variogram. However, the distribution still did not conform to the assumption of normality, and so we used the method of Cressie & Hawkins (1980) for a more robust estimation of the variogram for this type of data. The computing formula is a modified version of Equation 2.4:

$$\hat{\gamma}(\mathbf{h}) = \frac{1}{2} \frac{\left\{ \frac{1}{m(\mathbf{h})} \sum_{j=1}^{m(\mathbf{h})} |z(\mathbf{x}_j) - z(\mathbf{x}_j + \mathbf{h})|^2 \right\}^4}{0.457 + \frac{0.494}{m(\mathbf{h})} + \frac{0.045}{m^2(\mathbf{h})}} \quad (2.5)$$

where trend was present in the data, as it was for silt content, we incorporated it in a mixed model of fixed and random effects in the REML estimation of the variogram (Webster & Oliver, 2007).

We mapped the variables across the field by ordinary kriging at points on a 1 m grid and then contoured the predictions in ArcMap (ESRI Inc.). For the variables in which we identified trend and used REML to obtain the variogram we used universal kriging to take the trend into account.

## 2.4 Results

Individuals of *A. myosuroides* were found in 95% of the 0.5 m<sup>2</sup> quadrats. In total, 3917 *A. myosuroides* seedlings were counted with a mean density of 28.8 per quadrat (Table 2.1). However, the spatial distribution of *A. myosuroides* plants varied throughout the field and had a strongly skewed distribution. A model was fitted to try and normalize the data. The best fit was obtained for logarithms of the data with an offset of 0.6 added before logging. This removed the skew from the data, but revealed a bimodal distribution. When the field was divided into two at the site of the old field boundary, both populations then fitted a negative binomial distribution; a distribution associated with aggregated populations (Gonzalez-Andujar & Saavedra, 2003). The soil properties measured were all approximately normal in distribution.

The accumulated components of variance show clear spatial structure in both *A. myosuroides* counts and the soil properties measured (Figure 2.4). At fine scales the variance components estimated by REML analysis are similar to the expected variance

**Table 2.1.** Summary statistics of species counts and environmental variables in the field in Harpenden.

Variate	Mean	Minimum	Maximum	Standard deviation	Skew
<i>A. myosuroides</i> (individuals per quadrat)	28.80	0	326	51.01	3.022
Cultivation depth (cm)	24.90	17.1	30.0	2.74	0.132
Gravimetric water content in top 10 cm (%)	25.63	21.8	30.0	1.86	0.582
Gravimetric water content 10–28 cm depth (%)	23.83	19.3	31.0	2.19	0.546
Organic matter (% wet weight)	4.53	3	6	0.65	0.452
Available phosphorus (mg l <sup>-1</sup> )	24.70	11	54.4	8.36	1.271
pH	6.90	6.13	7.79	0.28	0.245
Sand (% wet weight)	32.10	17	51	4.85	0.413
Silt (% wet weight)	39.51	25	50	4.27	0.0788
Clay (% wet weight)	28.39	23	39	3.00	0.846
Volume of Stones (%)	19.17	4.444	38.89	6.67	0.507
Mass of Stones (g)	172.5	20.3	387.0	75.43	0.131

obtained from the variogram. However, in most cases the variogram reaches a sill at lag distances greater than the maximum distance in the nested design. The functions chosen as models for the variograms were those that best fitted in the least squares sense (Table 2.2).

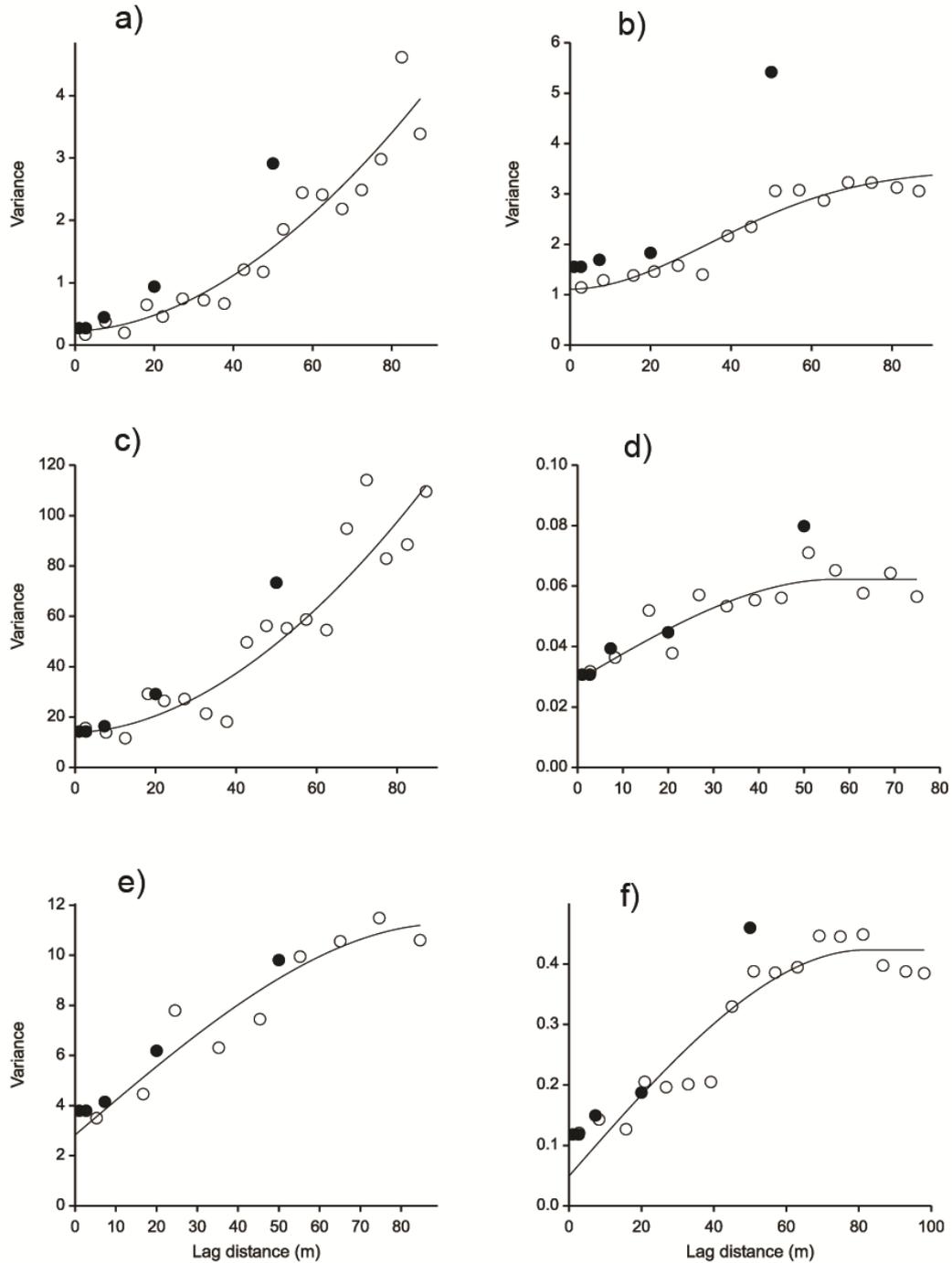


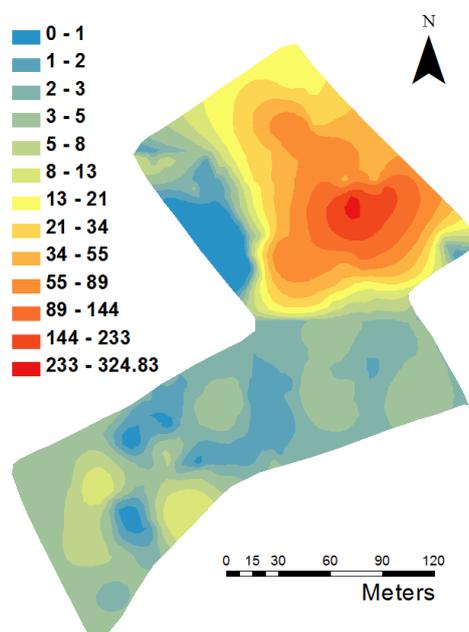
Figure 2.4. Figure legend on page 42.

**Figure 2.4.** (Figure on page 41.) Accumulated components of variance with all negative components of variance set to zero (closed discs) and variograms (open circles) for (a) *A. myosuroides*, (b) gravimetric water content in the top 10 cm of soil, (c) available phosphorus, (d) pH, (e) clay content, (f) organic matter. The lags have been binned over all directions and incremented in steps of 6 m. The components of variance plotted at 50 m are calculated from the top level (1) of the design and so encompass all distances greater than 50 m. The solid black line shows the models fitted.

**Table 2.2.** Variogram models fitted to describe the spatial structure in selected measured variables. \*For *A. myosuroides* logarithms of the data are used with an offset of 0.6 added before logging. \*\*The stable model uses an exponent of 0.95.

Variate	Type of Model	Nugget	Range	Distance Parameter	Sill	Exponent	Linear Term
<i>A. myosuroides</i> *	Power	0.229	-	-	-	1.837	0.00101
Gravimetric water content in top 10 cm	Stable**	1.110	-	20.23	2.367	-	-
Available phosphorus	Power	13.95	-	-	-	1.837	0.0266
pH	Spherical	0.02890	57.0	-	0.0333	-	-
Clay	Spherical	2.83	91.0	-	8.42	-	-
Organic matter	Spherical	0.0492	82.03	-	0.3742	-	-

The map of *A. myosuroides* in Figure 2.5 was produced by combination of two separate krigings, one for each half of the field thereby taking into account the bimodal distribution of the weed counts. It shows a large concentration of weeds in the northern part of the field with only a few seedlings in the southern part of the field. The kriged maps of the soil properties (Figure 2.6) show each soil property has a unique spatial distribution. Some of the maps, for example water content (Figure 2.6 a) and pH (Figure 2.6 c), show some accord with *A. myosuroides* distribution (Figure 2.5).



**Figure 2.5.** Kriged maps of *A. myosuroides* individuals (per 0.5 m<sup>2</sup>). The model fitted to the experimental variogram of the data is used to provide the best unbiased predictions at points that were not sampled.

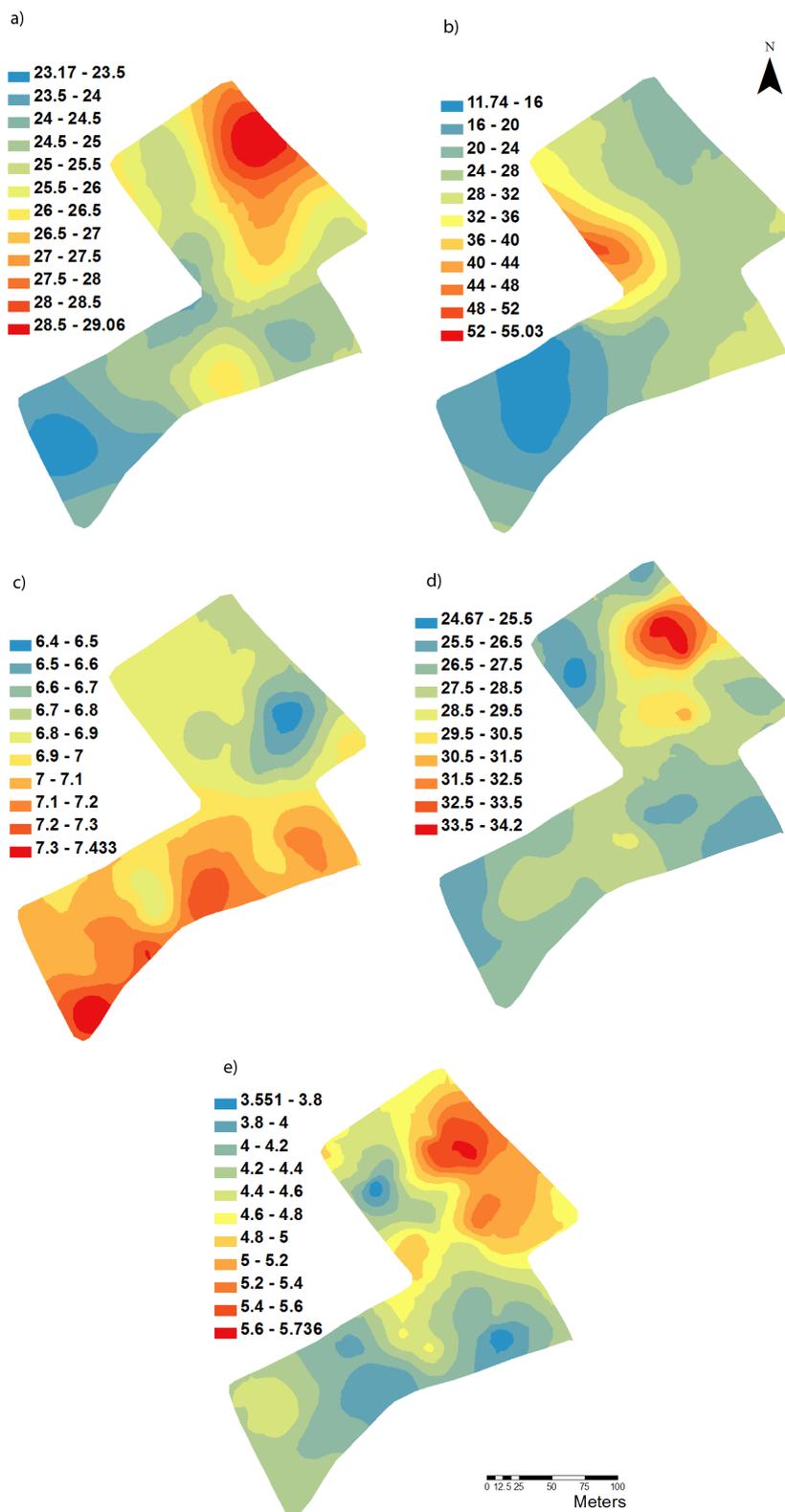


Figure 2.6. Figure legend on page 45.

**Figure 2.6.** (Figure on page 44.) Kriged maps of (a) gravimetric water content in the top 10 cm of soil (%), (b) available phosphorus ( $\text{mg l}^{-1}$ ), (c) pH, (d) clay content (%) and (e) organic matter (%) in soil. In all cases the models fitted to the experimental variograms of the data are used to provide the best unbiased predictions at unsampled points.

The statistically significant REML model terms were generally found at the coarsest scales studied here (Table 2.3) where the covariance terms ( $C_i^{u,v}$ ) for each scale ( $i = 1, 2, \dots, k$ ) were set to zero in turn in the REML analysis to test for significance in their contribution to the model.

**Table 2.3.** Estimated variance components for environmental variables at multiple spatial scales together with the covariance component with *A. myosuroides* at those scales. Covariances that contributed significantly to the model fitted by REML ( $P < 0.05$ ) are marked \*. Random terms are denoted by lv to signify the level of the hierarchical design, with lv 1 representing the highest level of the design (separate designs across the field) and so corresponds to distances of greater than 50 m and lv 2–5 correspond to distances of 20 m, 7.3 m, 2.7 m and 1 m respectively. All negative estimates for variance components were found not to be statistically significantly different from 0.

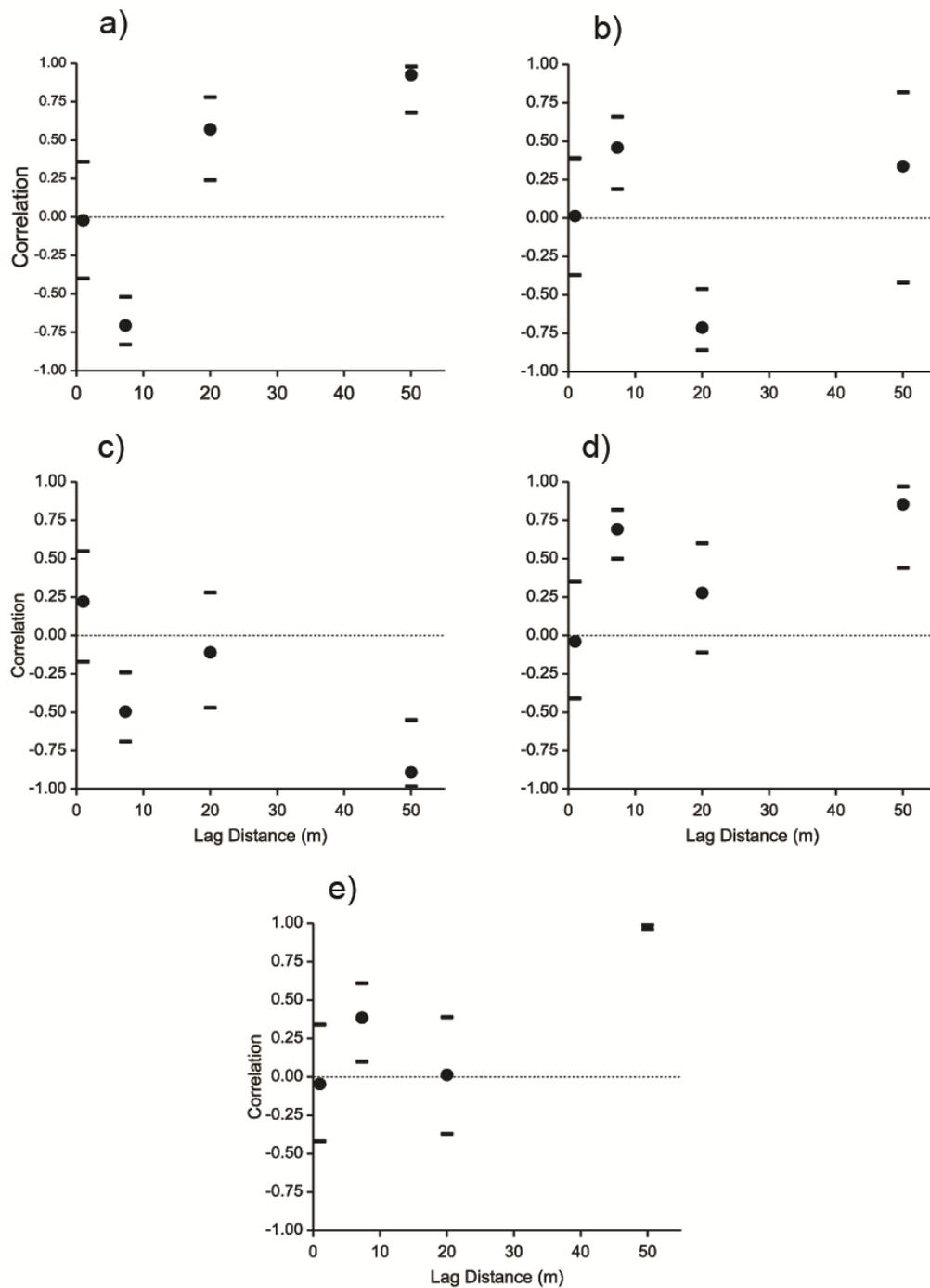
Environmental Variable	Random Term	Estimated variance component for environmental property	Estimated variance component for <i>A. myosuroides</i> counts	Estimated covariance component for environmental property and <i>A. myosuroides</i>
Gravimetric water content in top 10 cm	lv1	3.603	1.995	2.480*
	lv1.lv2	0.1239	0.4850	0.1401
	lv1.lv2.lv3	0.1481	0.1802	-0.1154
	lv1.lv2.lv3.lv4	-0.2244	-0.00972	0.1387
	Residual Variance: lv1.lv2.lv3.lv4.lv5	1.559	0.2620	-0.01321
Available phosphorus	lv1	43.93	1.976	3.150
	lv1.lv2	12.88	0.4960	-1.803*
	lv1.lv2.lv3	2.008	0.1720	0.2699
	lv1.lv2.lv3.lv4	-1.638	-0.01731	-0.1812
	Residual Variance: lv1.lv2.lv3.lv4.lv5	13.98	0.2701	0.02844

**Table 2.3** continued overleaf

Table 2.3 continued

Environmental Variable	Random Term	Estimated variance component for environmental property	Estimated variance component for <i>A. myosuroides</i> counts	Estimated covariance component for environmental property and <i>A. myosuroides</i>
pH	lv1	0.03577	1.981	-0.2368*
	lv1.lv2	0.005170	0.4940	-0.005534
	lv1.lv2.lv3	0.008005	0.1753	-0.01073
	lv1.lv2.lv3.lv4	-0.004391	-0.02287	-0.01073
	Residual Variance:			
	lv1.lv2.lv3.lv4.lv5	0.03132	0.2748	0.02055
Clay	lv1	3.692	1.952	2.294*
	lv1.lv2	1.986	0.4936	0.2752
	lv1.lv2.lv3	0.2887	0.1690	0.1531
	lv1.lv2.lv3.lv4	-0.5752	-0.02259	0.005526
	Residual Variance:			
	lv1.lv2.lv3.lv4.lv5	3.904	0.2765	-0.03997
Organic matter	lv1	0.2749	1.963	0.728*
	lv1.lv2	0.03782	0.493	0.00194
	lv1.lv2.lv3	0.02876	0.1725	0.02713
	lv1.lv2.lv3.lv4	-0.01191	-0.01379	0.008752
	Residual Variance:			
	lv1.lv2.lv3.lv4.lv5	0.1193	0.2677	-0.00817

Pearson correlation coefficients between *A. myosuroides* counts and the soil properties are generally weak (Table 2.4). These take all of the data into account without regard to spatial scale. From these results we might conclude that there are only weak relations between the density of *A. myosuroides* and the environmental properties measured. However, once the correlations are calculated using the nested design structure stronger relations are revealed at particular scales (Figure 2.7). Often, significant terms in the REML model (Table 2.3) correspond with strong correlations between the *A. myosuroides* count and the soil property (Figure 2.7), reiterating the likelihood of there being a relation between the weed count and the soil property at that scale.



**Figure 2.7.** Graphs of correlations at the various scales of the nested sampling design between *A. myosuroides* and (a) water content in the top 10 cm of soil, (b) available phosphorus, (c) pH, (d) clay content, and (e) organic matter. Correlations are shown as discs with horizontal bars indicating 95% confidence intervals. The correlations plotted at 50 m are calculated from the top level (1) of the design and so encompass all distances greater than 50 m.

**Table 2.4.** Pearson correlation coefficients between *A. myosuroides* counts and soil properties measured taking all data into account. Two-sided tests of correlations different from zero are marked \* where significant ( $P < 0.05$ ).

Variate	Pearson correlation coefficient between <i>A. myosuroides</i> and the measured variate
Cultivation depth	-0.008
Gravimetric water content in top 10 cm	0.482*
Gravimetric water content 10–28 cm depth	0.491*
Organic matter	0.527*
Available phosphorus	0.023
pH	-0.475*
Sand	0.135
Silt	-0.384*
Clay	0.328*
Volume of stones	0.050
Mass of stones	0.031

### 2.4.1 Optimizing the Design

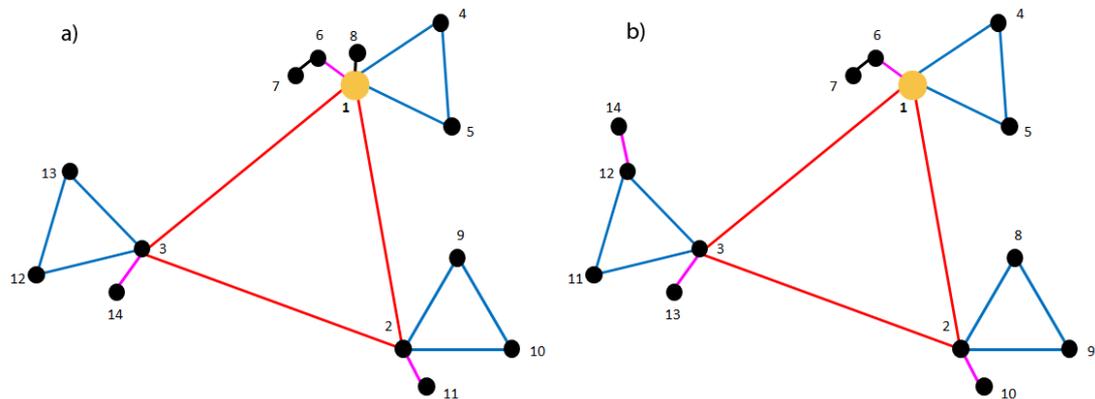
At the beginning of our study we had no prior information about the distribution of the variance across scales. Therefore the nested design we used was based on the assumption of equal variances at all scales. As we now know the components of variance for *A. myosuroides* seedling counts at all scales (Table 2.5), the sampling design can be optimized as described by Lark (2011). This allows sampling to be focused on the scales that contribute most to the total variance. To achieve this all components of variance must be positive, and so in this example the component of variance for the 4th level is set equal to the minimum positive variance. The optimized design is shown in Figure 2.8 a.

Because of the relations observed at the coarse scale between *A. myosuroides* and most of the soil properties we investigated a wider set of scales increasing exponentially from 1 m at level 5 to 40 m at level 2. This meant the use of distances of 1 m, 3.5 m, 11.5 m and 40 m within the design at each main station. Estimates of the components of variance at each of these distances were taken from the model fitted to the variogram for *A. myosuroides* counts. The component of variance for the top level of the design was set so that the variances had the same sum as the original REML estimates for this

**Table 2.5.** Results of REML analysis for log transformed *A. myosuroides* counts. Random terms are denoted by lv to signify the level of the hierarchical design, with lv 1 representing the highest level of the design (separate designs across the field) and so corresponds to distances of greater than 50 m and lv2–5 correspond to distances of 20 m, 7.3 m, 2.7 m and 1 m respectively.

Random term	Estimated variance component	Estimated standard error	Effective degrees of freedom
lv1	1.9759	1.0951	8
lv1.lv2	0.4916	0.2126	18
lv1.lv2.lv3	0.1759	0.0816	34.22
lv1.lv2.lv3.lv4	-0.0176	0.0609	33.19
Residual variance:			
lv1.lv2.lv3.lv4.lv5	0.2700	0.0679	31.6

field. The design was then optimized for these estimated components of variance. The optimized design at the coarser scales is shown in Figure 2.8 b.



**Figure 2.8.** Optimized nested designs with sampling points at vertices (labelled 1–14) as they would appear in the field for (a) the original scales as used in the field in Harpenden (Red = 20 m, Blue = 7.3 m, Purple = 2.7 m, Black = 1 m) with optimized topology according to the estimated components of variance from the REML analysis of *A. myosuroides* counts, (b) the new coarser scales (Red = 40 m, Blue = 11.5 m, Purple = 3.4 m, Black = 1 m) with optimized topology according to the estimated components of variance from the model fitted to the variogram of *A. myosuroides* counts.

## 2.5 Discussion and Conclusions

Both the hierarchical analysis and the estimated variogram of the *A. myosuroides* counts revealed clear spatial structure in the data with observations at short separations showing greater similarity than observations separated by larger distances. Each of the soil variables we measured also had its unique spatial structure which was visible in both the variograms and the components of variance (see Figure 2.4). This means that we must recognize the importance of variation at several spatial scales. Within the literature on weed patches, there is a lack of consistency in observed relations with abiotic variables. For example Walter *et al.* (2002) found a weak negative relation between *Poa annua* L. (annual meadow grass) and organic matter content, whereas Andreasen *et al.* (1991) found a strong positive relation between the two. This lack of consistency may be due to their different sampling scales. Walter *et al.* (2002) sampled on a 20 m  $\times$  20 m grid whereas Andreasen *et al.* (1991) randomly selected sample locations within a field. This illustrates the need for more rigorous statistical methods to account for processes operating at different scales.

Despite weak Pearson correlations for all the data (Table 2.4), covariances and correlations between *A. myosuroides* counts and soil properties showed some strong correlations at various scales. In most instances the separations that significantly contributed in the REML analyses were the largest of those studied here ( $>50$  m) indicating relations between soil properties and *A. myosuroides* counts occur across the whole field. This is a potentially interesting result in terms of the practical management implications (as we explain below) and warrants further investigation into the scale-dependent relations between *A. myosuroides* and soil properties. In terms of experimental and analytical methodology it is particularly important to note how uncorrelated variation between two variables at finer scales can obscure scientifically interesting, and practically important, relations exhibited at coarser scales if one were only to examine the overall correlation between variables. The nested sampling scheme and associated analysis set out in this paper are necessary if this problem is to be avoided in experimental studies of the factors affecting weed distribution.

However, other fine-scale relations not revealed by significant terms in the REML model did appear in the correlations between the weed and soil properties. For example, there are strong positive relations observed at the two coarsest scales between

*A. myosuroides* and water content. However, at 7.3 m there is a negative relation between these two variables, indicating that a different process operates over these smaller distances. So, although *A. myosuroides* establishes most readily in the wettest part of the field, within that wet part establishment is better in the relatively dry parts of it. Similarly for available phosphorus, despite the negligible Pearson correlation between *A. myosuroides* and phosphorus, at 20 m there is a significant negative covariance in the REML model, yet at the 7.3 m scale the correlation is positive. This may be explained by depletion of available phosphorus in areas of high weed density (Webster & Oliver, 2007, pp. 220 and 227–228).

We have shown how by nested sampling and hierarchical analysis by REML one can reveal the spatial scale(s) on which weed infestations vary and correlate with soil factors in an economical way. We have also shown how, once one has estimates of components of variance, one can improve a design for future survey without adding substantially to the cost.

These estimates of the components of the variance could be estimated from other more readily available sources of information. For example the farmer might know something, in a qualitative way, of where and on what spatial scales weeds infest their fields or the investigator might have access to aerial photography or satellite images that show patchiness in crops or soil and which could guide them in designing a sampling scheme. Our methodology is generic and can be used to look at relations between any continuous variable assumed to be related to weed distribution and any weedy variable, whether species distribution or total weed density. We should expect the spatial dependency of soil and weed interactions revealed by the analysis to be context specific. However, ongoing work is seeking to validate the robustness of the relations between soil and *A. myosuroides* patches that emerged from our case study.

This paper has demonstrated how scale-dependent relations between weed density and soil properties can be examined by appropriate sampling and analysis. The case study shows that such scale-dependence can occur. It also shows that the nested method may allow us to identify relations that occur at certain scales but which would be obscured by uncorrelated variations at other scales if the variables were examined using only the overall correlation for data on a simple random sample. This methodology should be applied to a range of fields with contrasting soil conditions and management strategies, over several seasons, in order to identify scale-dependent relations between

soil and weeds which could form a basis for a robust strategy for controlling weeds according to the spatial variation of the soil.

Identifying the soil properties that most consistently affect the distribution of *A. myosuroides* in a field could have practical application if the scale at which the soil and weeds are correlated is appropriate for site-specific management (as is suggested by our results). Farmers often aim to minimize heterogeneity within individual fields so that they can treat each field as if it were uniform. Nevertheless, they recognize that there will be some variation within their fields and often have considerable knowledge of that spatial variation (Heijting *et al.*, 2007). Now, with modern technology they can vary their treatment applications accordingly (Lutman *et al.*, 2002). Patchy distributions of weeds are particular examples of such heterogeneity. In principle, farmers should be able to control the weeds with herbicide where the weeds occur and avoid using herbicide where they are absent or too few to be of consequence. Although research is being pursued into detection of weed seedlings (e.g. Giselsson *et al.*, 2013), most current systems, especially for grass weeds, rely on mapping weeds at maturity to guide spraying decisions in the following crop. Knowing the relations between weeds and soil could underpin these approaches by identifying “weed vulnerable zones”, based on thresholds of soil variables, for example clay content, in the field where the weeds might persist or spread. These areas could be sprayed as buffers around existing patches to insure against individuals escaping control. Ultimately, if sufficiently robust models of weed spatial distribution could be developed (incorporating thresholds of soil properties) soil maps could be used as the basis for weed patch spraying decisions. Furthermore, if the coarse-scale relations observed here are found to be common across additional fields it is more likely that farmers would adopt variable management at these scales than precision spraying at fine scales.

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## Chapter 3

# Defining the Habitat Niche of Black-grass (*Alopecurus myosuroides*) at the Field Scale.

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In the previous chapter I described a nested sampling design which allows the study of scale-dependent relationships between weed distributions and environmental properties. By using this sampling design I could partition the variance into scale-dependent components, and so find strong scale-dependent correlations between *A. myosuroides* and soil properties. Other researchers failed to identify such strong relationships due to their failure to consider scale in their studies. In order to address my first hypothesis that the within-field spatial distribution of *A. myosuroides* is associated with the spatial distribution of environmental variables at scales appropriate for management, I implemented the designs described in Chapter 2 in four additional fields: The initial design, assuming equal variance at all scales, was used in the case-study field (Harpenden) and one additional field (Radbrook), whilst the design optimised to focus sampling

effort at the scales discovered to be of most importance in the field in Harpenden (as described in Chapter 2) was implemented in a further three fields (Redbourn, Ivinghoe and Haversham).

The following work is under review with Weed Research and was submitted in July 2017. It describes the implementation of the nested sampling design in five fields and the results obtained. I describe the spatial variation in *A. myosuroides* and various soil properties within the fields and explore scale-dependent relationships between *A. myosuroides* and environmental properties following the methodology outlined in Chapter 2. I also describe a general relationship across the five fields, determined by a regression type analysis using REML. This allowed me to determine the suite of environmental variables that best predict *A. myosuroides* counts across all fields. These environmental variables, that I have found to be the most important within-field determinants of the spatial distribution of *A. myosuroides* will be explored further in Chapters 4 and 5 where I look at their effects on the life-cycle and the management of this species.

### **3.1 Summary**

The distribution of *A. myosuroides* in fields is patchy. The locations of these patches can be influenced by the environment. This presents an opportunity for precision management through patch spraying. We surveyed five fields on various types of soil using a nested sampling design and recorded both *A. myosuroides* seedlings in autumn and heads in summer. We also measured soil properties at those sampling locations. We found that the patches of heads within a field were smaller than the seedling patches, suggesting that techniques for patch spraying based on maps of heads in the previous season could be inherently risky. We also found that the location of *A. myosuroides* patches within fields can be predicted through their relation with environmental properties and that these relations are consistent across fields on different soil types. This improved understanding of the relations between soil properties and *A. myosuroides* seedlings could allow farmers to use pre-existing, or suitably supplemented soil maps already in use for the precision application of fertilizers as a starting point in the creation of herbicide application maps.

## 3.2 Introduction

*Alopecurus myosuroides* Huds. (black-grass) is one of the most common grass weeds of winter cereals in north-west Europe (Holm *et al.*, 1997) and is particularly problematic in the UK. *Alopecurus myosuroides* has a high reproductive rate and competes strongly with cereal crops (Maréchal *et al.*, 2012). When mature, *A. myosuroides* plants produce large amounts of seeds, and so small failures in control can lead to rapid population growth and dense infestations. For many farmers, the main option for control of *A. myosuroides* and other weeds in the UK is the application of herbicides. These are often heavily relied upon as the sole method of control. In 2015, in the UK, 4,200 tonnes of herbicides were applied to cereal crops (FERA, 2017). Many farmers apply herbicides uniformly across individual fields and use on average six herbicidal active substances in a season for an arable crop (Garthwaite *et al.*, 2014). Despite this heavy reliance on multiple chemical controls, many farmers are experiencing waning effectiveness owing to the evolution of herbicide resistance (Heap, 2017). These farmers are seeking alternative methods of weed management.

In addition to the need to delay or avoid the evolution of herbicide resistance, there are two further reasons to reduce herbicide use. First, agrochemicals can have negative impacts on the environment. Their inappropriate use can lead to contamination of surface water, ground water and the atmosphere (Garibay *et al.*, 2001), this may contribute to loss of biodiversity, loss of ecosystem function, and contamination of drinking water. Second, an increasing number of regulations are being placed on herbicides, and so, by reducing their use, farmers would become less reliant on individual active ingredients that could be withdrawn in the future. The benefits of minimizing herbicide use are therefore multiple: selection pressure would be reduced, and the effective life of some active ingredients would be prolonged, environmental concerns would be reduced, and there would be less reliance on this singular method of control, thereby encouraging greater adoption of integrated weed management programs. One opportunity for reducing herbicide inputs is to spray only those areas of the field where weeds are a problem (site-specific weed management).

*Alopecurus myosuroides*, like many weed species, grows in patches within fields. These patches can vary in size and shape (Cardina *et al.*, 1997; Dieleman *et al.*, 2000; Walter *et al.*, 2002; Heijting *et al.*, 2007), nevertheless these patches can be fairly stable,

with core areas of *A. myosuroides* patches moving only 3–4 m over several years (Lutman *et al.*, 2002). Patchiness can lead to many inefficiencies in weed management, as often farmers spray whole fields if average weed densities exceed some threshold, whereas there may be large parts of their fields that do not require spraying. In this situation, blanket spraying wastes time, energy and chemical (Cardina *et al.*, 1997). Advances in global positioning technology and precision sprayers now make it possible to manage weeds at a much finer spatial resolution than was previously possible. There are two methods through which such forms of patch management can be achieved (Walter *et al.*, 2002). The first is using treatment maps. These can be created from manually sampled data on weed distributions. These maps can sometimes be of inadequate quality, often because the sampling on which they are based was too sparse (Metcalf *et al.*, 2016 (Chapter 2)). The second approach is through real-time detection of weeds with optical sensors—usually detecting mature weeds in the previous cropping season to inform spraying decisions in the following year. This approach is still in development, and whilst already feasible it is not yet at the stage of widespread commercialization (e.g. Murdoch *et al.*, 2010, 2014).

Despite the numerous benefits of introducing patch spraying as a form of weed management, it is not being readily taken up as a standard management tool. There may be several reasons for this, perhaps the most difficult to counter being the inherent conservativeness of farmers when it comes to weed control. Given the consequences of a control failure, the concept of leaving some areas of the field unsprayed is currently seen as an unacceptable risk.

There is some indication that the patchy distribution of *A. myosuroides* is related to the similar variation in the soil (Holm *et al.*, 1997; Lutman *et al.*, 2002, Murdoch *et al.*, 2014). The principle of the ecological niche tells us that a plant will thrive in the environment most favourable to it, and so we expect that environmental variation will play a role in the location of weed patches in the context of the spatial aggregation that is an emergent property of random seed dispersal (Paice *et al.*, 1998). Our lack of understanding of what determines this field-scale habitat niche of this important species is currently preventing the implementation of site-specific management based on that knowledge. Understanding where weeds are in a field and what is determining their spatial distribution might not only reduce input costs but also lead to the more accurate application of other control practices where needed (Dieleman *et al.*, 2000), including

variable seed rates and fertilizer applications. If we can understand how patches relate to soil, we might explain the observed distribution on *A. myosuroides* in each field but also define the potential habitat into which it could spread. In so doing, we could build insurance into any patch spraying protocol. This would also allow the use of existing or supplemented soil maps.

Previous investigators who have attempted to link *A. myosuroides* density and soil properties have limited their scope, only sampling at a single scale (e.g. Dunker & Nordmeyer, 1999 and 2000; Lutman *et al.*, 2002). This has led to discrepancies in conclusions that can be drawn, with conflicting results from different studies. Metcalfe *et al.* (2016 (Chapter 2)) proposed a solution to resolve discrepancies in field studies. They found that relations that occur at certain scales could be obscured by uncorrelated variations at other scales if only the overall correlation were calculated from all the data from a simple random sample. They successfully demonstrated in one field that relations between *A. myosuroides* and soil properties are dependent on the spatial scale and different results can be obtained from different sampling scales.

We applied this approach to five winter wheat fields with contrasting soil types over several seasons to investigate the relationships between soil properties and both *A. myosuroides* seedling counts and head counts. We set out to test three hypotheses:

1. the response of counts of seedlings and heads are similar, which if true means patch-spraying can be based on head counts recorded in the previous growing season,
2. variance within fields of the distribution of *A. myosuroides* depends on relationships with soil properties at specific spatial scales, and,
3. these relationships are similar from field to field.

By addressing these hypotheses, we hope to establish whether farmers could use soil maps in the management of *A. myosuroides* and whether the scale of these relationships is appropriate for precise management of the weed.

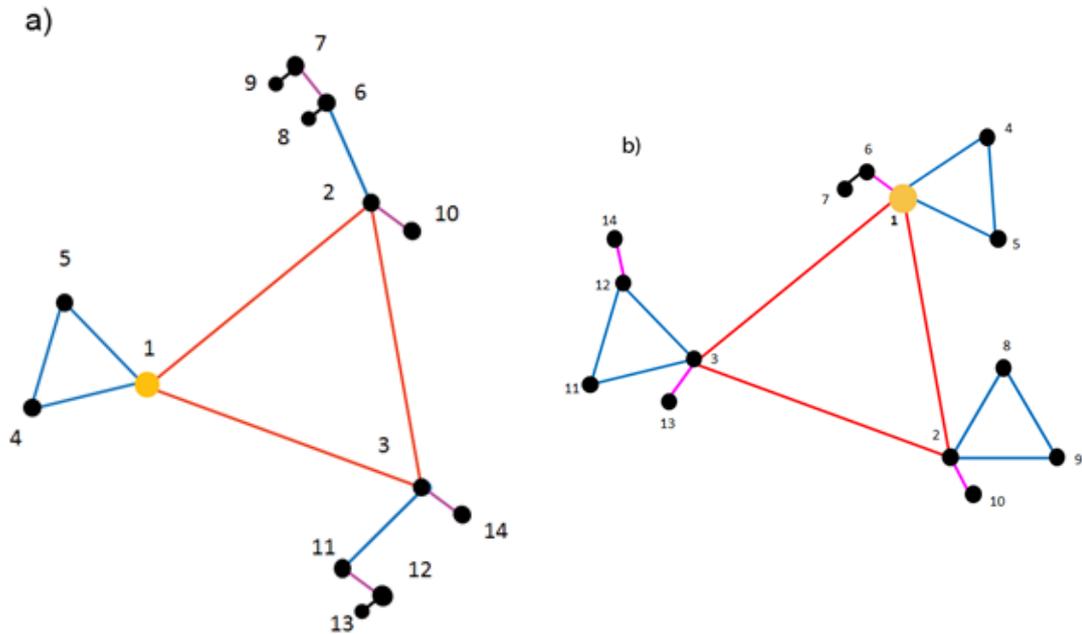
### 3.3 Materials and Methods

#### 3.3.1 Field Sites

We chose five sites with a range of soil types. Each site consisted of one field, which was in commercial winter wheat production in the season of study. All fields were in the south-east of England (the main centre of *A. myosuroides* distribution) and reported by the farmers to have patchy *A. myosuroides* populations. The fields were separated by a minimum distance of 5.3 km and maximum of 65.6 km. Here, we refer to the fields by their location in Radbrook (Berkshire), Harpenden (Hertfordshire), Redbourn (Hertfordshire), Ivinghoe (Buckinghamshire) and Haversham (Buckinghamshire). Radbrook was studied in the 2012–13 season, Harpenden in the 2013–14 season, Redbourn and Ivinghoe in the 2014–15 season and Haversham in the 2015–16 season.

#### 3.3.2 Nested Sampling

We used an unbalanced nested sampling scheme as described by Metcalfe *et al.* (2016 (Chapter 2)). The design is organized hierarchically with five levels. Each level corresponds to a specific scale of study with level 1 defining the coarsest scale in each study and level 5 the finest (Figure 3.1). Figure 3.1 shows the organization of sample sites associated with one main station of the nested design. The level-one variation is represented by differences between the groups of sample sites associated with each main station in each field. Note that while the distances between points are constrained by the design the directions are randomized independently in each main station. We sampled at nine such clusters in each field. Sampling sites were nested hierarchically in groups associated with each main station per the distances indicated in Table 3.1. We used an initial design with five scales (detailed in Table 3.1) in the first two fields at Radbrook and Harpenden. Based on the results from these two fields we optimized the design, as described by Metcalfe *et al.* (2016 (Chapter 2)), for use in the other three fields. This optimized design used coarser scales (Table 3.1) to try to capture better some of the coarse-scale variation in *A. myosuroides* observed in the first two fields. To map the distribution of *A. myosuroides* and associated soil properties by kriging we added ten more sampling points in each field to fill the larger gaps in the coverage and thereby diminish the errors in prediction.



**Figure 3.1.** Nested sampling designs used in (a) Harpenden and Radbrook, (b) Redbourn, Ivinghoe and Haversham. Vertices are labelled as the numbers 1–14. The yellow disc indicates the main station of the motif. Designs were separated by distances from level one. Red lines represent nodes spaced at level two of the design, blue lines indicate level three, purple lines link points at level four and black lines represent level five.

**Table 3.1.** Scales used at each level of the nested sampling design in each field. The nested design consists of five levels as described by Metcalfe *et al.* (2016 (Chapter 2)). Level one represents the coarsest scales and with each subsequent level, the scale is made finer. The design was refined after the first year’s results from Harpenden and Radbrook, explaining the difference in the scales from the remaining study fields.

Level of nested sampling design	Scale / m				
	<i>Harpenden</i>	<i>Radbrook</i>	<i>Redbourn</i>	<i>Ivinghoe</i>	<i>Haversham</i>
1	50+	50+	60+	60+	60+
2	20	20	40	40	40
3	7.3	7.3	11.5	11.5	11.5
4	2.7	2.7	3.4	3.4	3.4
5	1	1	1	1	1

We located the positions for each main station at level 1 of the design by GPS (Topcon/Trimble, 2 cm accuracy). Each subsidiary sampling point was located by its distance and orientation from the main station by tape measure and compass. To define the sample support, we placed square quadrats (0.5 m<sup>2</sup>) on the ground with their south-west vertices at the sampling point.

### 3.3.3 Weed Counts

We counted *A. myosuroides* seedlings within each quadrat in late autumn, while the plants were at the one- to two-leaf stage. For fields where pre-emergence herbicides were to be applied by the farmer, we placed plastic sheets over the sample quadrats for up to 24 hours to prevent herbicide reaching the sampling area. Seedling counts were obtained at Harpenden, Redbourn, Ivinghoe, and Haversham, but were not done at Radbrook as the field was included in the study too late for seedlings to be assessed.

We counted *A. myosuroides* heads within the month prior to harvest of the wheat crop. We included in the count any heads within the vertical area directly above the quadrat. We disregarded any heads falling outside the quadrat irrespective of whether the plant originated inside the quadrat. Head counts were obtained at Harpenden, Radbrook, Redbourn, Ivinghoe. Because of very dense *A. myosuroides* at Haversham, extensive lodging of the crop made heads counts inaccurate.

### 3.3.4 Soil Analyses

We sampled the soil in early winter, following prolonged rainfall, when we presumed soil moisture to be at field capacity. We took two soil cores from each quadrat with a half-cylindrical auger of diameter 3 cm to a depth of 28 cm. We measured the gravimetric water content in layers 0–10 cm and 10–28 cm by loss on oven-drying at 105°C for all sites except Radbrook. At Radbrook we calculated a measure of volumetric water instead from theta probe measurements of the soil surface layers. Other variables were analysed by SOYL (Newbury, UK) on samples pooled from the two cores within each quadrat. Organic matter was measured by loss on ignition. Available phosphorus (P) was measured in a sodium bicarbonate extract at pH 8.2. The pH was measured in water, and soil texture (particle-size distribution) was determined by laser diffraction.

We did not measure organic matter and available phosphorus at Radbrook.

### **3.3.5 Topography**

Elevation data (LIDAR) were downloaded from data.gov.uk for each field (except Ivinghoe where the data were unavailable) at a 1 m resolution. We converted this into aspect and slope information using ArcGIS spatial analyst. To include these as one variate in our analyses we computed the solar energy received throughout one year following methods outlined by Frank & Lee (1966).

### **3.3.6 Analysis**

We calculated summary statistics and Pearson correlation coefficients for all data. Note, however, that due to the use of the nested sampling design this does not give an unbiased estimate of the correlation because it ignores the dependency structure imposed by the sampling. The first level of the analysis was done at the level of individual fields (variograms and kriging, principal components analysis, and nested analysis). We then tested the hypothesis that these relationships were consistent across fields using all the data in a combined model (regression analysis).

#### **Variograms and Kriging**

To create maps of seedling densities, we estimated and modelled variograms from all data points from both the sampling design and the ten additional points to quantify the spatial structure in the variance of the measured variables. We did this using GenStat (Payne, 2013). We used ordinary kriging to predict the variables of interest across the field at points on a 1-m grid and then contoured the predictions in ArcMap (ESRI Inc.) to make maps.

#### **Principal Components Analysis**

To obtain an overall appreciation of the correlations among the soil properties and how the *A. myosuroides* counts fit into that structure we did principal components

analyses, as follows. We standardized the soil variables to mean=0 and variance=1, and effectively did the analysis on the correlation matrix,  $\mathbf{R}$ , for each field separately. We then computed the Pearson correlation coefficients between the component scores as

$$b_{ij} = a_{ij} \sqrt{\lambda_j / \sigma_i^2} \quad (3.1)$$

where  $a_{ij}$  denotes the  $i$ th element of the  $j$ th eigenvector and  $\lambda_j$  is the  $j$ th eigenvalue of matrix  $\mathbf{R}$ , and  $\sigma_i^2$  is the variance of the  $i$ th original soil variable. We plotted the coefficients  $b$  for the two leading components in unit circles and then added to the graphs the correlation coefficients between the *A. myosuroides* counts, sometimes regarded as “passive variables”, and the two leading components as described by Abdi & Williams (2010).

### **Nested Analysis**

The nested design structure allows the partitioning of the components of variance for both *A. myosuroides* and soil properties at each of the spatial scales studied. We did this using the residual maximum likelihood (REML) estimator as described by Metcalfe *et al.* (2016 (Chapter 2)). Following partitioning of the components of variance at the different spatial scales, we estimated the correlations between *A. myosuroides* and the soil properties at each scale where the estimated components of variance were positive. We calculated confidence intervals (95%) for the correlations by Fisher’s  $z$ -transform, with degrees of freedom appropriate to the number of sampled pairs at the corresponding level of the design. Where the confidence intervals excluded zero we determined the correlation to be statistically significantly different from zero.

### **Regression Analysis**

We tested the hypothesis that the relationships between the variance in *A. myosuroides* density and soil properties quantified at the individual field scale were consistent across the five fields. In this type of analysis, it is important that all terms are independent. As our three soil texture variables (sand, silt, and clay) sum to 100%, they cannot be independent. We used the additive log-ratio transform (Aitchison, 1986) to create two independent variables (the log of the ratio of silt to sand, and the log of the ratio of clay

to sand). We also removed the soil moisture content below 10 cm from this analysis as it was strongly correlated with surface soil moisture content, which is more likely to be recorded in soil surveys.

We did a regression analysis using REML where the field was included as a random term. We included all environmental properties as main effects. For this analysis, we considered only the first-order model for soil properties to retain sufficient degrees of freedom for the analysis. Terms were selected using backwards elimination according to the largest P-value given by an F test when that term was dropped. The best model was chosen when all remaining terms gave significant values ( $P \leq 0.05$ ) for an F test when dropped from the model.

We also looked at incorporating the spatial autocorrelation in *A. myosuroides* numbers into this regression analysis by including the field location and variogram parameters as random effects. Again, terms were selected using backwards elimination according to the largest P-value given by an F test when that term was dropped. We also considered the possibility of using maximum likelihood in the place of REML as this method allows us to compare AIC values across models with different fixed effects. For this model backward elimination was also used for term selection.

### 3.4 Results

*Alopecurus myosuroides* was present in all five fields. Numbers of *A. myosuroides* seedlings were highest in Haversham and lowest in Radbrook (Table 3.2). The fields spanned a range of soil types and the soil properties we measured varied substantially from one field to another. There were also different levels of within-field variation in soil properties (Table 3.2). For example, pH was highest in Ivinghoe and lowest in Radbrook but Redbourn showed the greatest variation.

**Table 3.2.** Summary statistics for *A. myosuroides* counts and soil properties measured in each field.\* indicates missing data.

Variate	Mean	Minimum	Maximum	Standard Deviation	Skewness
<i>Harpenden</i>					
<i>A. myosuroides</i> seedling counts (per 0.5 m <sup>2</sup> quadrat)	28.8	0	326	51.0	3.022
<i>A. myosuroides</i> head counts (per 0.5 m <sup>2</sup> quadrat)	18.6	0	266	48.4	3.361
Gravimetric water content in top 10 cm (%)	25.63	21.8	30.0	1.86	0.5796
Gravimetric water content 10–28 cm depth (%)	23.83	19.3	31.0	2.19	0.5529
Organic matter (% wet weight)	4.53	3.0	6.0	0.65	0.4515
Available phosphorus (mg l <sup>-1</sup> )	24.70	11.0	54.4	8.30	1.2711
pH	6.90	6.1	7.8	0.28	0.2452
Sand (% wet weight)	32.1	17	51	4.9	0.413
Silt (% wet weight)	39.5	25	50	4.3	0.079
Clay (% wet weight)	28.4	23	39	3.0	0.846
<i>Radbroom</i>					
<i>A. myosuroides</i> seedling counts counts (per 0.5 m <sup>2</sup> quadrat)	*	*	*	*	*
<i>A. myosuroides</i> head counts (per 0.5 m <sup>2</sup> quadrat)	4.2	0	95	14.3	4.250
Volumetric water content in top 10 cm (%)	18.02	12.6	27.1	2.98	0.4134
Gravimetric water content 10–28 cm depth (%)	*	*	*	*	*
Organic matter (% wet weight)	*	*	*	*	*
Available phosphorus (mg l <sup>-1</sup> )	*	*	*	*	*
pH	5.87	4.9	6.9	0.45	0.1530
Sand (% wet weight)	33.5	15	53	7.9	0.137
Silt (% wet weight)	60.1	44	75	6.2	-0.078
Clay (% wet weight)	6.4	3	12	2.1	0.306

Table 3.2 continued overleaf

Table 3.2 continued

Variate	Mean	Minimum	Maximum	Standard Deviation	Skewness
<i>Redbourn</i>					
<i>A. myosuroides</i> seedling ) counts (per 0.5 m <sup>2</sup> quadrat)	12.8	0	129	20.4	2.658
<i>A. myosuroides</i> head counts (per 0.5 m <sup>2</sup> quadrat)	11.0	0	107	21.3	2.623
Gravimetric water content in top 10 cm (%)	20.63	16.3	25.2	1.71	0.2640
Gravimetric water content 10–28 cm depth (%)	20.80	16.8	25.0	1.96	0.3887
Organic matter (% wet weight)	4.67	3.4	6.9	0.73	0.6735
Available phosphorus (mg l <sup>-1</sup> )	25.93	12.6	44.6	6.85	0.4422
pH	7.09	5.6	8.3	0.65	-0.1315
Sand (% wet weight)	28.4	9	46	5.5	0.175
Silt (% wet weight)	44.3	34	68	5.0	1.053
Clay (% wet weight)	27.3	15	38	4.2	0.537
<i>Ivinghoe</i>					
<i>A. myosuroides</i> seedling counts (per 0.5 m <sup>2</sup> quadrat)	3.3	0	84	10.2	5.929
<i>A. myosuroides</i> head ) counts (per 0.5 m <sup>2</sup> quadrat)	6.1	0	172	22.5	5.817
Gravimetric water content in top 10 cm (%)	22.34	18.7	24.8	0.91	-0.6583
Gravimetric water content 10–28 cm depth (%)	21.06	18.2	23.9	1.07	-0.0209
Organic matter (% wet weight)	4.73	3.6	5.7	0.43	0.0294
Available phosphorus (mg l <sup>-1</sup> )	14.29	9.6	23.4	2.58	0.6174
pH	8.11	7.7	8.5	0.14	0.0927
Sand (% wet weight)	22.1	11	47	8.2	1.335
Silt (% wet weight)	28.8	11	38	4.2	-0.720
Clay (% wet weight)	49.1	33	63	5.7	-0.632

Table 3.2 continued overleaf

Table 3.2 continued

Variate	Mean	Minimum	Maximum	Standard Deviation	Skewness
<i>Haversham</i>					
<i>A. myosuroides</i> seedling counts (per 0.5 m <sup>2</sup> quadrat)	63.6	0	488	111.9	2.030
<i>A. myosuroides</i> head counts (per 0.5 m <sup>2</sup> quadrat)	*	*	*	*	*
Gravimetric water content in top 10 cm (%)	22.49	17.4	28.2	2.13	0.3929
Gravimetric water content 10–28 cm depth (%)	20.92	15.9	26.0	1.93	0.1560
Organic matter (% wet weight)	4.26	3.1	5.8	0.53	0.3124
Available phosphorus (mg l <sup>-1</sup> )	9.07	4.8	16.0	2.43	0.7981
pH	7.21	6.5	7.9	0.29	-0.3882
Sand (% wet weight)	44.9	23	62	8.6	-0.508
Silt (% wet weight)	29.6	22	38	3.7	-0.039
Clay (% wet weight)	25.5	16	40	5.4	0.952

The relationships between *A. myosuroides* and soil properties as expressed by Pearson correlations were strong for water, organic matter and texture (Table 3.3). Other soil properties, such as available phosphorus, were only weakly correlated with *A. myosuroides* (Table 3.3). The relationships between *A. myosuroides* seedling counts and soil properties were stronger and more consistent across fields than between soil properties and head counts.

### 3.4.1 Variograms and Kriging

Generally, the distribution of *A. myosuroides* heads within the fields showed the same pattern as for seedlings, but in many instances the patches were smaller (Figure 3.2). The distribution in all fields was patchy (Figure 3.2) with all fields having some quadrats free of *A. myosuroides*.

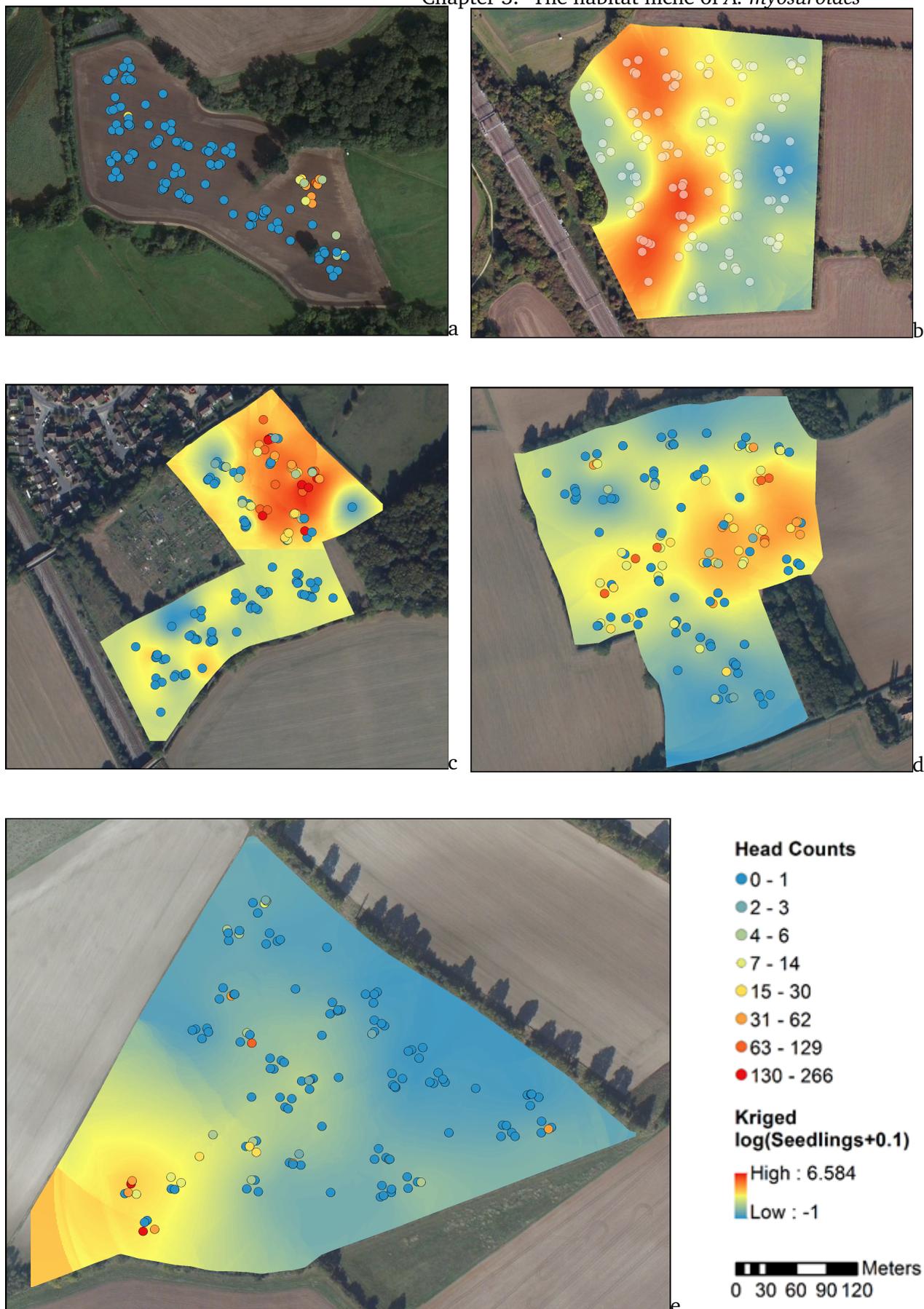


Figure 3.2. Figure legend on page 72.

**Table 3.3.** Pearson correlation coefficients between *A. myosuroides* seedling and head counts and soil properties in each field. This analysis takes all data into account, ignoring the nested sampling structure. Two-sided tests of correlations different from zero are marked \* where significant ( $P \leq 0.05$ ). †Gravimetric water content was measured except for Radbrook where we measured volumetric water content). ‡indicates missing data.

Soil Property	Harpenden		Radbrook		Redbourn		Ivinghoe		Haversham	
	Seedlings	Heads	Seedlings	Heads	Seedlings	Heads	Seedlings	Heads	Seedlings	Heads
Gravimetric water content in top 10 cm (%)†	0.482*	0.279*	‡	0.292*	0.321*	0.172	0.101	0.080	0.616*	‡
Gravimetric water content 10-28 cm depth (%)	0.491*	0.342*	‡	‡	0.519*	0.280*	-0.172	-0.051	0.448*	‡
Organic matter (% wet weight)	0.527*	0.309*	‡	‡	0.462*	0.269*	-0.080	0.108	0.349*	‡
Available phosphorus ( $\text{mg l}^{-1}$ )	0.023	0.041	‡	‡	-0.132	-0.184*	-0.132	-0.011	0.029	‡
pH	-0.475*	-0.310*	†	0.337*	0.017	-0.062	-0.001	-0.094	0.112	‡
Sand (% wet weight)	0.135	0.139	‡	-0.189*	0.049	0.007	-0.235*	-0.157	-0.253*	‡
Silt (% wet weight)	-0.384*	-0.264*	‡	0.124	-0.320*	-0.144	0.034	0.061	0.176*	‡
Clay (% wet weight)	0.328*	0.152	‡	0.348*	0.324*	0.165	0.326*	0.188*	0.280*	‡

**Figure 3.2.** (Figure on page 70.) Maps showing the sampling locations (circles) in each of the five fields: a) Radbrook b) Haversham, c) Harpenden, d) Redbourn, e) Ivinghoe. Where the circles are filled, the colour indicates the number of heads counted in a 0.5 m<sup>2</sup> quadrat at that sampling location. Where the field is filled, the colour represents the kriged values for log (seedling counts + 0.1) in a 0.5 m<sup>2</sup> quadrat at each sampling location. The kriging was conducted using ordinary kriging based on the variogram fitted for that field.

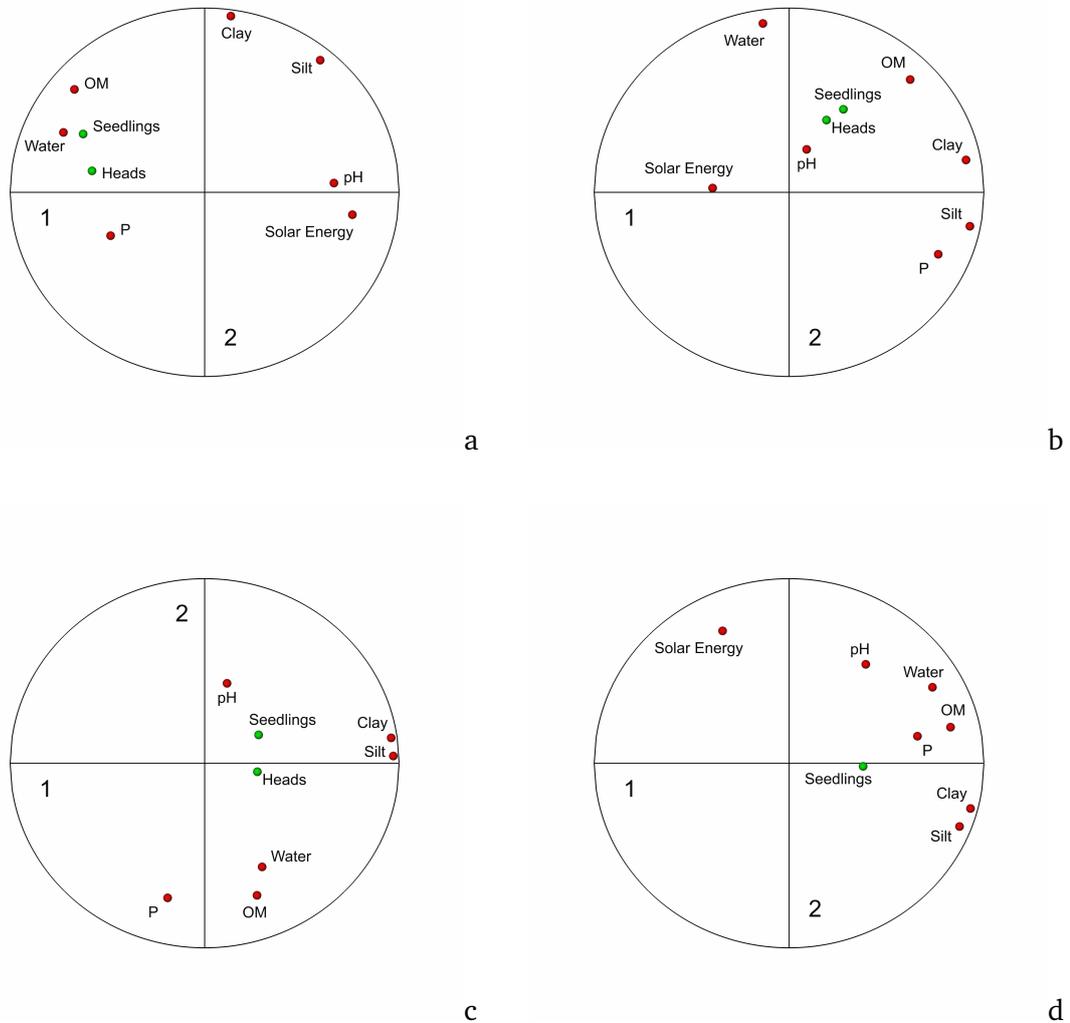
We can see in the kriged maps that there is some accord between *A. myosuroides* distribution (Figure 3.2) and soil moisture (Supplementary Figure S3.1), organic matter (Supplementary Figure S3.2), clay content (Supplementary Figure S3.3) and pH (Supplementary Figure S3.4). It is also notable that in Radbrook and Ivinghoe, where we see the fewest *A. myosuroides* (Table 3.2) we also find the driest soil, and the most extreme values of soil pH (Supplementary Figures S3.3 and S3.4).

### 3.4.2 Principal Components Analysis

Within each field, we observed consistent covariation in soil properties (Figure 3.3). The largest amount of variation (PC1) in soil properties within a field was accounted for by soil texture and water. Soil pH explained an additional source of variation and generally corresponds with PC2 (Figure 3.3).

### 3.4.3 Nested Analysis

The scale-dependent analysis of the nested design revealed much stronger correlations between *A. myosuroides* and particular soil properties than did the Pearson correlation. At medium to coarse scales, there are significant positive correlations between organic matter and the number of *A. myosuroides* seedlings in all fields except for Ivinghoe, which also had the least intra-field variance for this soil property (Table 3.4). These relationships are particularly strong at coarse scales. Relationships were weaker for heads, and the only significant correlation between organic matter and heads was found in Harpenden at level 2 of the design (Table 3.4). The patterns observed relating organic matter and *A. myosuroides* at Ivinghoe differ from the other four fields. In this field, the



**Figure 3.3.** Principal component analysis on soil properties measured in four study sites (Radbrook did not have sufficient soil properties measured to warrant analysis by PCA): (a) Harpenden, (b) Redbourn, (c) Ivinghoe, and (d) Haversham. The first two principal components are shown here in unit circles with the correlation coefficient for each soil property shown with a red disc. The correlations for the *A. myosuroides* counts are passively projected onto the principal component plot (without being included in the analysis) to show how they relate to the soil properties.

**Table 3.4.** Scale-dependent correlations between *A. myosuroides* counts and soil properties. Correlation coefficients shown in bold are significantly different from zero †indicates where a negative variance component was fitted using REML as part of the nested analysis, these were found to be not significantly different from zero. ‡indicates that no model could be fitted using REML. \*Indicates missing data.

Scale	Harpenden		Radbrook		Redbourn		Ivinghoe		Haversham	
	Seedlings	Heads	Seedlings	Heads	Seedlings	Heads	Seedlings	Heads	Seedlings	Heads
<i>Soil Organic Matter</i>										
1	<b>0.99</b>	†	*	*	<b>0.69</b>	‡	-0.08	0.21	<b>0.90</b>	*
2	0.01	<b>-0.62</b>	*	*	<b>0.68</b>	‡	†	†	0.22	*
3	<b>0.39</b>	-0.05	*	*	<b>0.28</b>	‡	<b>-0.32</b>	0.03	<b>0.62</b>	*
4	†	†	*	*	†	‡	<b>-0.34</b>	-0.05	0.06	*
5	-0.05	-0.12	*	*	†	‡	†	0.19	†	*
<i>Soil water content in the top 10 cm (gravimetric water content was measured except for Radbrook where we measured volumetric water content)</i>										
1	<b>0.93</b>	<b>0.91</b>	*	0.54	0.55	<b>0.92</b>	0.44	<b>0.73</b>	0.65	*
2	<b>0.57</b>	0.07	*	†	†	†	†	†	<b>0.71</b>	*
3	<b>-0.71</b>	<b>0.33</b>	*	†	†	†	†	†	<b>0.84</b>	*
4	†	†	*	†	†	0.32	-0.22	0.21	<b>0.99</b>	*
5	<b>0.93</b>	<b>0.91</b>	*	0.54	0.55	<b>0.92</b>	0.44	<b>0.73</b>	0.65	*

Table 3.4 continued overleaf

Table 3.4 continued

Scale	Harpenden		Radbrook		Redbourn		Ivinghoe		Haversham	
	Seedlings	Heads	Seedlings	Heads	Seedlings	Heads	Seedlings	Heads	Seedlings	Heads
<i>Soil pH</i>										
1	<b>-0.89</b>	‡	*	<b>0.80</b>	0.03	-0.32	-0.17	<b>-0.88</b>	‡	*
2	-0.11	‡	*	†	0.25	-0.02	†	†	‡	*
3	<b>-0.49</b>	‡	*	†	-0.21	†	†	†	‡	*
4	†	‡	*	-0.17	†	<b>0.79</b>	<b>-0.34</b>	†	‡	*
5	0.22	‡	*	-0.12	†	†	†	-0.36	‡	*
<i>Soil clay content</i>										
1	<b>0.85</b>	<b>0.83</b>	*	0.61	<b>0.71</b>	‡	0.45	0.44	0.55	*
2	0.28	0.05	*	†	0.32	‡	†	†	0.22	*
3	<b>0.69</b>	0.25	*	<b>0.96</b>	<b>0.46</b>	‡	†	†	<b>0.24</b>	*
4	†	†	*	<b>0.52</b>	<b>-0.88</b>	‡	<b>0.36</b>	-0.06	0.08	*
5	-0.04	-0.18	*	-0.35	†	‡	†	0.25	†	*

overall variation in organic matter was smaller than in the other fields.

Across all fields, we see a broad correspondence between *A. myosuroides* seedling and head numbers and moisture content (Figures 3.2 and S3.1, and Table 3.3). This is confirmed by significant correlations at multiple scales for both seedlings and heads (Table 3.4).

In Harpenden, we found a significantly strong negative correlation between *A. myosuroides* seedlings and pH at coarse and medium scales (Table 3.4). Ivinghoe, where the pH was similar showed a significant negative relationship at the 3.4–11.5 m scale as well as a coarse-scale negative relationship with *A. myosuroides* heads (Table 3.4). However, in Radbrook and Redbourn, where the soil is generally more acid we observe significant positive correlations (Table 3.4). These results suggest a non-linear, unimodal, relationship between pH and *A. myosuroides* and that a slightly acidic pH is the most favourable for *A. myosuroides*.

Soil texture is reported to be an important influence on the presence of *A. myosuroides* (Lutman *et al.*, 2002), and our data supported this. There were significant positive correlations between clay and *A. myosuroides* at all sites with larger positive correlations tending to be at coarse scales (Table 3.4). The compositional nature of the relationship between the three texture variables means that we observed negative counterparts in silt and sand. We observed similar relationships emerging for heads, yet these tended to be much smaller correlation coefficients indicating the link between soil texture and *A. myosuroides* was weaker for heads than for seedlings (Table 3.4).

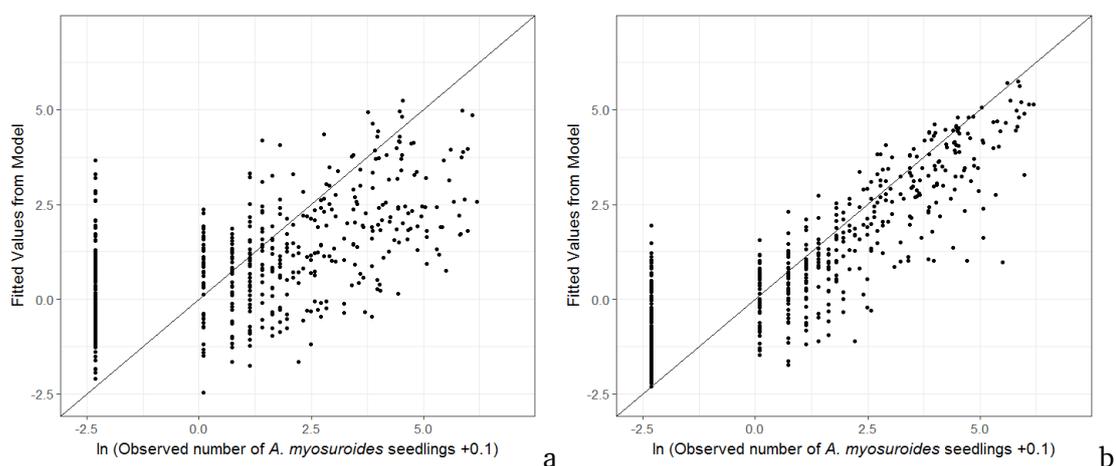
#### 3.4.4 Regression analysis

When we considered all study sites together, as part of the regression analysis, a suite of soil properties including texture, water, and topography (as defined by solar energy) (Table 3.5) provided a good prediction of *A. myosuroides* seedling densities (Figure 3.4 a). If we account for the autocorrelation in *A. myosuroides* seedling densities by fitting a spherical variogram with a nugget of 2.207, range 105.4 m and a sill of 1.298 then our predictive capability was further improved (Figure 3.4 b). Despite the autocorrelation giving us improved predictive power, there is still scope for soil properties to be used to improve the prediction with soil pH, water and topography significantly contributing

**Table 3.5.** Terms selected in a regression type analysis using REML to predict *A. myosuroides* seedling densities from soil properties. The non-spatial model has only field location as a random effect, whereas the spatial model allows the estimation of a variogram as a random effect. Here a spherical variogram with a nugget of 2.207, range of 105.4 m and a sill of 1.298 was fitted.

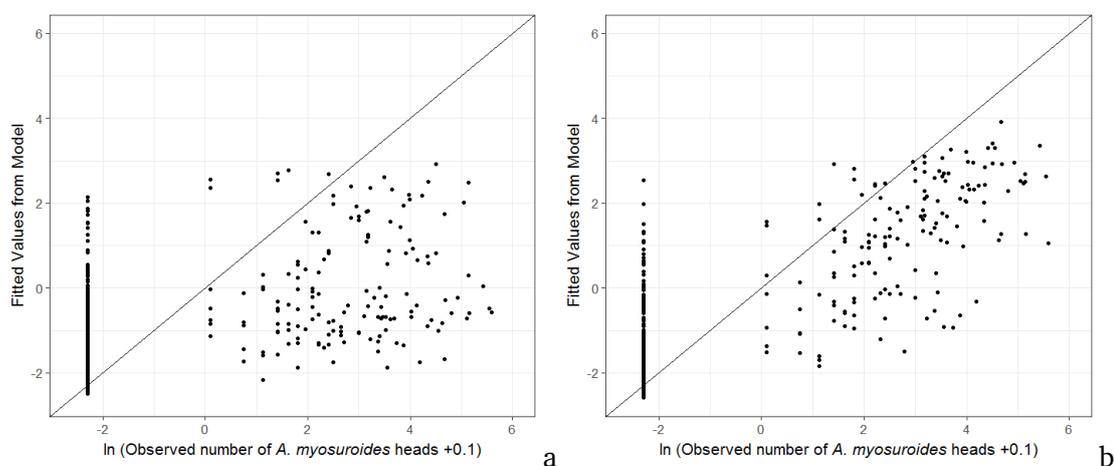
Term	Effect	S.E.
<i>Non-spatial model</i>		
Constant	0.9030	1.04080
Log(clay:sand)	2.131	0.6132
Log(silt:sand)	-1.524	0.6082
Gravimetric water content — top 10 cm	0.3806	0.06015
Solar energy	-0.002344	0.0004427
<i>Spatial model</i>		
Constant	0.5675	0.62214
pH	0.6692	0.28583
Gravimetric water content — top 10 cm	0.2429	0.05839
Solar energy	-0.001669	0.0007076

to this model (Table 3.5), the same soil property terms were selected by the maximum likelihood approach, albeit with different effects due to the different type of model fitted.



**Figure 3.4.** Scatter plots showing the relationship between the observed *A. myosuroides* seedling densities and the values predicted by the regression model. The non-spatial model (a) incorporates the fixed effects as listed in Table 3.5 and field location as a random effect. The spatial model (b) also incorporates an estimation of the variogram to describe spatial auto-correlation in the *A. myosuroides* seedling counts.

Despite our ability to predict the density of *A. myosuroides* seedling populations from soil properties fairly accurately, our experience for heads was less promising (Figure 3.5). Again, the addition of information on the autocorrelation in head numbers (spherical model, nugget = 2.470, range = 122.3 m, sill = 1.136) reduces the need for as many soil properties to be considered (Supplementary Table S3.1). However, the predictive power is still poorer than for seedling densities (Compare Figure 3.5 with Figure 3.4) and the model fitted using maximum likelihood incorporates different terms. The discrepancy between these two approaches indicates the lack of fit in these models and brings doubt as to the usefulness of using soil properties in the prediction of head densities.



**Figure 3.5.** Scatter plots showing the relationship between the observed *A. myosuroides* head counts and the values predicted by the regression model. The non-spatial model (a) incorporates the fixed effects as listed in Supplementary Table S3.1 and field location as a random effect. The spatial model (b) also incorporates an estimation of the variogram to describe spatial auto-correlation in the *A. myosuroides* seedling counts.

### 3.5 Discussion

Our results confirm that the distribution of *A. myosuroides* seedlings in the autumn can be patchy in fields growing winter wheat for commercial purposes (Figure 3.2). We also found that the distribution of seed heads in the summer is a contraction of the initial *A. myosuroides* patch (Figure 3.2). This observation is contrary to our first hypothesis and so highlights a problem associated with current methods of patch spraying, which map *A. myosuroides* heads in the summer to guide herbicide application of seedlings in the following season (Walter *et al.*, 2002). If the contraction of patches is due to the

environment, then this does not pose a risk to the farmer. However, if the contraction of patches during the growing season is due to effective management measures in the intervening period then there is a risk the patches could expand again if those same measures are not implemented in the following season.

We have shown that, generally, there are strong correlations between *A. myosuroides* and soil properties that are associated with the first principal component of soil variation, namely soil texture, organic matter and water (Figure 3.3, Table 3.3). These primary sources of variation could be linked to *A. myosuroides* seedling numbers by correlation at multiple spatial scales (Table 3.4) and so may be useful predictors of patch location. In addition, pH, a secondary source of within-field variation in soil (Figure 3.3), could also be linked to *A. myosuroides* seedling counts, and so measurement of this in the field is likely to provide more information than measurement of additional soil properties linked to the main source of variation (PC1 in Figure 3.3).

When trying to predict *A. myosuroides* densities from soil properties we found that the best predictors came from a regression model that considered the underlying auto-correlation in *A. myosuroides* seedling numbers (Figure 3.4). In this model, information about soil improved that prediction with soil moisture and pH being of importance (Table 3.5). These two soil properties represent the two main sources of variation in soil within the five fields (Figure 3.3). Solar energy was also important indicating that the topography of the fields is important for the distribution of *A. myosuroides* seedlings (Table 3.5). Areas of the fields with consistently dense *A. myosuroides* were characterised by large clay and organic matter content with a slightly acid pH and received little solar energy (meaning they were less prone to drying out).

Our findings were reasonably consistent across all five fields, which covered a few growing seasons and soil types. This provides some support for our third hypothesis and indicates that the patterns observed here may be general. The strongest relationships between soil properties and *A. myosuroides* we found were in Redbourn and Harpenden, the fields with intermediate infestation. Where infestation was highest (Haversham) and particularly low (Ivinghoe and Radbrook) there were weaker correlations between *A. myosuroides* numbers and soil properties. This indicates that the relationship between *A. myosuroides* and soil properties might depend on plant density. Where *A. myosuroides* densities are low the relationship with the soil was weak as the patch may not have reached all areas suitable for growth. Where densities are high there might be spill over

out of the optimal parts of the field as seed production is so great it is likely that some seed will germinate and the plants will grow even outside their optimal environment. In this outcome, it is unlikely that patch spraying would be recommended as more effective field scale weed management is required.

The use of soil properties in the prediction of patch locations looks promising as it is fairly consistent across fields and seasons, particularly if we consider the incorporation of spatial autocorrelation in the prediction of seedling numbers. Where our predictive power is poorest seems to be in the prediction of areas with no *A. myosuroides* seedlings (Figure 3.4). However, our model is more likely to predict that there will be *A. myosuroides* present when there is none—making it risk averse and so more likely to be useful to farmers.

The scale-dependent correlations that provide the strongest links between *A. myosuroides* counts and soil properties are most often at coarse scales (Table 3.4). This is particularly pertinent for weed management as it is a scale that is useful for the farmer. Most machinery currently available on farm operates at scales of 20 m or greater and so it is helpful to know that this is a relevant scale for management, if patch spraying were to be implemented based on soil maps.

### 3.5.1 Conclusions

We have shown that it is more important for farmers to be able to target patches of *A. myosuroides* seedlings than the mature plants as the seedlings cover a greater part of the field. Seedling patches can be predicted by relationships with soil properties, and these relationships are consistent across fields. This improved understanding of the relationship between soil and *A. myosuroides* seedlings could allow pre-existing, or supplemented soil maps already in use for the precision application of fertilisers to be a useful starting point in the creation of herbicide application maps.

## 3.6 Acknowledgements

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## Chapter 4

# The Effect of the Abiotic Environment on the Life-Cycle of Black-grass (*Alopecurus myosuroides*)

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In the field, I observed associations between *A. myosuroides* and several soil properties (Chapters 2 and 3). I have shown that these associations are scale-dependent and are relatively consistent across fields (Table 3.4 in Chapter 3). There could be many reasons for these associations between *A. myosuroides* distributions and soil properties. The soil may have both direct and indirect effects on the weed itself, as well as the herbicides used to control the weed. In this chapter I consider the direct effects of the environment on the weed, whilst Chapter 5 focuses on the effect of soil properties on pre-emergence herbicide efficacy. Here I test my second hypothesis that soil organic matter, moisture and pH affect the life-cycle of *A. myosuroides* from germination to seed return. These soil properties represent some of the main components of the within-field

soil variation identified as important in Chapter 3. I studied the effect of changing these soil properties in pot experiments on the life-cycle of *A. myosuroides*. I studied several processes within the *A. myosuroides* life-cycle, including germination, phenology, biomass production and seed production. I also included crop competition in one of my experiments. Some parts of what is written below, namely those concerning soil pH, were published in *Aspects of Applied Biology* **134** 145-150 in February 2017.

## 4.1 Summary

In-field studies have identified associations between *A. myosuroides* and soil properties particularly organic matter, texture and soil moisture content with a secondary relationship with pH. To give an insight into the mechanisms underlying these correlations, we explored these relationships further through pot experiments to investigate the effect of these three soil properties on various aspect of the life-cycle of *A. myosuroides* when grown in isolation and in competition with winter wheat (*Triticum aestivum* L.).

Soil organic matter had a significant impact on *A. myosuroides* germination and seed production, whilst few aspects of the *A. myosuroides* life-cycle were affected by altering soil pH in the pot experiment, suggesting that the results in the field may not be due to the change in pH alone but rather the interaction with other aspects of changing soil chemistry or structure. However, there was a small effect of soil pH on weed competitive ability when grown together with winter wheat. This may indicate that soil pH alone can have some influence on the location of *A. myosuroides* patches through an indirect effect of changing the competitive balance between the crop and the weed. These results indicate that the local soil environment can influence aspects of the life-cycle of *A. myosuroides* and as such may play an important role in determining the within-field distribution of this species.

This work also highlights the potential for the implementation of cultural control methods aimed at targeting different stages of the *A. myosuroides* life-cycle through changing soil husbandry or the use of crop cultivars that are more competitive over a range of soil conditions.

## 4.2 Introduction

Like any plant, the environment in which a weed is growing can be very important in determining its growth. The soil is a large component of the environmental variation experienced by the weed and it can have both direct and indirect effects on the growth and performance of the weed. Direct effects of the soil on the plant can be through changing the below-ground environment, where processes such as germination take place as well as affecting the uptake of resources from the soil which will, in turn, affect plant growth. The soil can also have indirect effects on the weed through changing competitive performance with the crop.

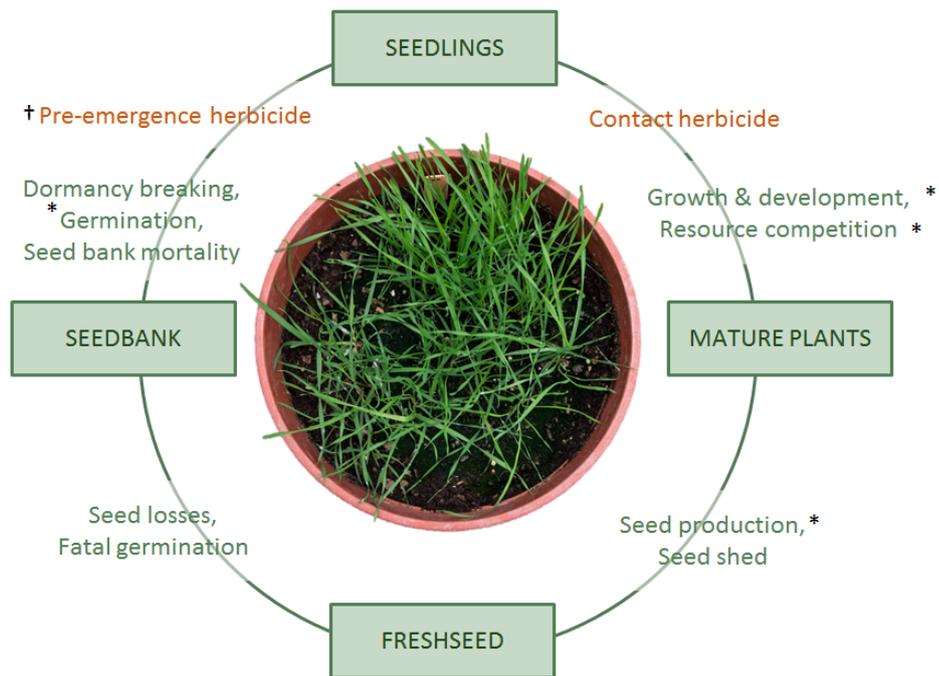
One aspect of a plant's life-cycle considered particularly susceptible to changes in environmental conditions is germination. A non-dormant seed has the capacity to germinate over a range of conditions when the temperature and light requirements of the species match with ambient conditions for sufficient time to allow the completion of germination. If just one environmental factor required for germination is unfulfilled germination will not occur (Finch-Savage & Leubner-Metzger, 2006). As germination is heavily associated with water availability it could be expected that on soil with high water storage capacity there may be greater levels of germination as the conditions would be more consistently favourable. Other factors associated with soil can also affect germination and seedling survival, such as fertility, salinity, compaction, tillage and surface residue (Forcella *et al.*, 2000). These changes in germination and seedling vigour have the potential to impose a large effect on competition with the crop (Weiner, 1986) and therefore the resulting population sizes.

Soil humidity and temperature are important in the early stages of *Alopecurus myosuroides* Huds. (black-grass) growth (Maréchal *et al.*, 2012). Soil conditions can affect competition between the weed and the crop for inorganic nutrients and other abiotic factors (Oerke, 2006) the intensity of this competition between crops and weed can depend on how resources are partitioned and how the niches of the crop and weed are differentiated. (Smith *et al.*, 2010). Given the shallow rooting structure of *A. myosuroides* it has been shown that it is more susceptible to droughting than wheat (Stratonovitch *et al.*, 2012) and that the magnitude of this effect is dependent on soil type, therefore we would expect that in areas more prone to droughting the wheat would have a competitive advantage.

In-field studies have identified associations between *A. myosuroides* and particular soil properties including organic matter and soil moisture content (e.g. Lutman *et al.*, 2002; Metcalfe *et al.*, 2016 (Chapter 2) and 2017 (Chapter 3)). Associations like these can often be explained by variation in the plant's strategy for water use, nutrient use or stress response. For example, *Avena fatua* L. (wild-oat) has a higher nitrogen use efficiency than wheat (Carlson & Hill, 1986), so in areas with higher soil nitrogen, its competitive effect is increased. Again, the different rooting structures of *A. myosuroides* and wheat allow them to exploit different pools of resource and may go some way to explaining the relationships observed in the field.

Some studies have observed an association between *A. myosuroides* and pH (e.g. Dunker & Nordmeyer, 2000; Metcalfe *et al.*, 2016 (Chapter 2), 2017 (Chapter 3)). Metcalfe *et al.* (2016, Chapter 2) found a modest correlation ( $R^2 = -0.475$ ) between pH and *A. myosuroides* seedling densities observed in 0.5 m<sup>2</sup> quadrats within a field in a nested sampling design separated by between 1 m and 50 m. However, an even stronger correlation was found ( $R^2 = -0.89$ ) when the data were analysed such that only the coarse scale correlations within the field were considered. This relationship could not be explained entirely through relations with other soil properties, indicating that pH may be independently affecting the within-field distribution of *A. myosuroides*. It is possible that the distribution of *A. myosuroides* within the field is partly determined by the influence of soil pH on the availability of many soil nutrients (Lucas & Davis, 1961). If the increased availability of certain nutrients provides a benefit for *A. myosuroides* plants, then these may have a competitive advantage relative to neighbouring plants such as winter wheat.

In-field studies, such as that by Metcalfe *et al.* (2017, Chapter 3) allow a comprehensive look at the effect of the soil on *A. myosuroides* distributions. However, separating out the effect of any individual soil property is extremely difficult due to the collocation of particular soil properties in space (Figure 2.6 in Chapter 2). Here we investigate the effect of changing soil properties on the growth of *A. myosuroides* in pots. We investigated the effect of soil organic matter, moisture, and pH, as well as crop competition on various stages of the life-cycle from germination to seed return (Figure 4.1). Through an increased understanding of how these soil properties affect the growth and competitive ability of *A. myosuroides* we aim to understand better the role played by variation in the soil in determining the within-field distribution of this species.



**Figure 4.1.** The life-cycle of *A. myosuroides*. Biological processes are shown in green and chemical interventions in orange. \*Represents aspects of the life-cycle that may be influenced by soil properties that are examined in this chapter (Chapter 4), whilst the impact of soil on pre-emergence herbicide efficacy (†) is examined in Chapter 5.

## 4.3 Methods

We ran three experiments in an outdoor hard standing area. For all experiments we used 25-cm pots placed on individual plastic saucers to prevent run off to neighbouring pots. We filled each pot with soil per the experimental design, outlined below. The area was netted and roofed to allow control over water input and protection from frost, whilst maintaining natural variation in temperature.

### 4.3.1 Plant material

We used seeds of *A. myosuroides* from a plot on the Broadbalk long-term experiment established at Rothamsted Research (Harpenden, UK) in 1843 that had never received any herbicides (Moss *et al.*, 2004). This population has been shown to be free of any evolved herbicide resistance. The seed was collected in 2012 and had been stored in darkness until use.

### 4.3.2 Experiment 1: Soil Organic Matter and Water Input

We studied the effect of changing soil organic matter (3 levels) and water input (2 levels) on the *A. myosuroides* life-cycle in the 2014–15 season. We had seven replicates of each treatment combination arranged in a randomized complete block design (a total of 42 pots). We mixed *A. myosuroides* seed ( $0.33 \pm 0.005$  g) into the top 2 cm of soil of each pot on the 24th October 2014 and assessed emergence as described below. In the winter (15th–18th January 2015), we thinned out each pot so that one *A. myosuroides* individual was left in the centre. We transplanted three wheat plants (2–3 leaf stage) into each pot spaced evenly around the centre (19th–22nd January 2015). We then allowed the plants to grow to maturity whilst maintaining the established watering treatments. No additional inputs were added to the soil to maintain the differences established by soil type. However, fungicides and insecticides were applied as required.

## Soils

We created three soils with varying organic matters, whilst maintaining other soil properties at relatively constant values by mixing sand, loam, and composted bark in different ratios. Samples of each soil mixture were tested by the laboratories at SOYL (Newbury, UK) to establish the amount of organic matter and pH (Table 4.1).

## Water Input

The second treatment was the amount of water input. There were two levels for this treatment: high (non-limiting) and low (limiting). We watered the pots at the high water input from above as required and by adding water to each saucer so that water availability was not limiting. In the low water treatment, we only watered intermittently at the first sign of wilting.

## Assessment

We recorded the number of emerged shoots every 2–4 days for four weeks until emergence had plateaued. We also measured the electrical conductivity of the soil using a theta probe to allow us to calculate the volumetric water content of each soil. Weather data were obtained from the meteorological station local to the experimental site. These two sets of data allowed the calculation of accumulated hydrothermal time:

$$\theta_{HT} = \sum [(\psi - \psi_b)(T - T_b)] \quad (4.1)$$

when the daily water potential ( $\psi$ ) and temperature ( $T$ ) were greater than the base water potential ( $\psi_b = -1.53$ ) and temperature ( $T_b = 0$ ) for *A. myosuroides* respectively. The values for these were taken from Colbach *et al.* (2002a and b) and were assumed to be constant, although for some species it has been shown that  $T_b$  can vary with  $\psi$  (Kebreab & Murdoch, 1999) .

We recorded the day of first flowering for each *A. myosuroides* plant. In mid-July, once all plants had flowered, we measured the height of the tallest tiller and the number of seed heads produced by the *A. myosuroides* plant in each pot. Once a seed head

**Table 4.1.** The volumetric composition of the three soil mixtures used in Experiment 1, their percentage organic matter measured by loss on ignition, and the measured pH of the soils.

Soil mixture	Coarse sand (% by volume)	Fine sand (% by volume)	Loam (% by volume)	Composted bark (% by volume)	OM (LOI % w/w)	pH
Low organic matter	35	35	22.5	7.5	1.93	7.16
Medium organic matter	20	20	45	15	2.37	7.00
High organic matter	0	0	75	25	6.15	7.00

was fully ripe we removed it from the plant to retain all seed before it was shed. In mid-August (13th–14th), we cut all biomass at ground level and separately recorded the dry weight of straw and seeds. We also calculated the proportion of the total biomass accounted for by seed.

### 4.3.3 Experiment 2: pH

We studied the effect of changing soil pH (2 levels) on *A. myosuroides* germination in late 2015. The experiment comprised a randomized block design with three pots for each pH treatment in each of seven replicate blocks (a total of 42 pots). We spread  $0.33 \pm 0.005$  g (approx. 150) seed evenly across the surface of each pot (3rd September 2015). Pots were watered as required.

#### Soils

We created two soils with contrasting pH, whilst maintaining other soil properties at relatively constant values. We chose to use a relatively acidic compost mixture as a starting point for the lower pH treatment (pH = 5.09). To create the higher pH treatment, we mixed lime into the soil at a rate equivalent to  $15 \text{ t ha}^{-1}$  to raise the pH to 6.95. Samples of each soil mixture were tested by the laboratories at SOYL (Newbury, UK) to establish the pH of each soil.

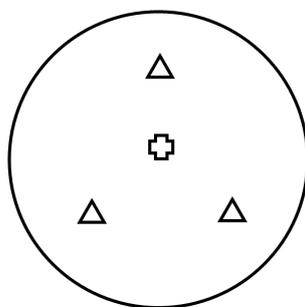
#### Assessment

We recorded the number of emerged shoots every 2–4 days for three weeks until emergence had plateaued.

### 4.3.4 Experiment 3: pH and Crop Competition

In Experiment 1 there were no pots with *A. myosuroides* growing in isolation, so we were unable to separate the direct effects of soil organic matter and watering on the weed life-cycle from the indirect effect of changing competitive performance with the crop. To address this in this pH study, we included an additional treatment of + / -

competition. We germinated *A. myosuroides* and winter wheat seeds and grew plants to the 3–4 leaf stage in the glass-house before transplanting them (8th March 2015) into pots containing compost at the two different pH levels (as in Experiment 2). Treatments included all six combinations of two soil pH levels, and each species individually or in competition. For the competition treatment, we grew *A. myosuroides* and wheat together in competition, and each species was also grown on its own. The plants were located within the pot as shown in Figure 4.2. The experiment comprised a randomized complete block design with one pot for each treatment combination in each of seven replicate blocks (a total of 42 pots). We then allowed the plants to grow to maturity. No additional inputs were added to the soil to maintain the differences established by soil type. However, fungicides and insecticides were applied as required.



**Figure 4.2.** Configuration of plants within pots. *Alopecurus myosuroides* is represented by the cross and wheat by the triangles. The position and number of plants of each species was consistent irrespective of whether they were grown in competition or alone.

### Assessment

We recorded the day of first flowering for each *A. myosuroides* plant and for the first wheat plant to flower in each pot. Once all plants had flowered, we measured the height of the tallest tiller and the number of seed heads produced for each plant of both species (25th July 2016). On the 22nd August 2016, we cut all biomass at ground level and separately recorded the dry weight of straw and heads for each species separately. We also calculated the proportion of the total biomass accounted for by seed. We calculated competitive performance of each species for each replicate by taking the total above-ground biomass of the plant grown in competition and dividing by the total biomass when grown in isolation on the same soil.

### 4.3.5 Data Analysis

For Experiments 1 and 2, we analysed the germination data by fitting a Gompertz curve (Equation 4.2) to all data from that trial. We restricted the origin to zero ( $A = 0$ ) but the  $B$ ,  $C$ , and  $M$  parameters could vary. We then looked at the change in fit when different curves were fitted for each treatment within the experiment (organic matter and water input in Experiment 1, and pH in Experiment 2) using an incremental F test (see supplementary material for tables).

$$y = A + Ce^{-e^{-B(x-M)}} \quad (4.2)$$

For Experiment 1 a two-way Analysis of Variance (ANOVA) was done to look at the influence of soil organic matter and watering on each life history trait measured. Soil organic matter included three levels (Low, medium and high) and water input consisted of two levels (low and high). For Experiment 2 a one way ANOVA was done to look at the effect of soil pH on total germination with two levels of pH (low and high). Finally, in Experiment 3 a general ANOVA was done to look at the effect of pH, competition and species on all life history traits measured. Again, pH had two levels (low and high), competition had two levels (with competition and without competition) and nested within each level of competition was species which also had two levels (*A. myosuroides* and wheat). All analyses were conducted in GenStat (Payne, 2013) and all ANOVA tables can be found in the supplementary material.

## 4.4 Results

### 4.4.1 Experiment 1: Soil organic matter and water input

#### Germination

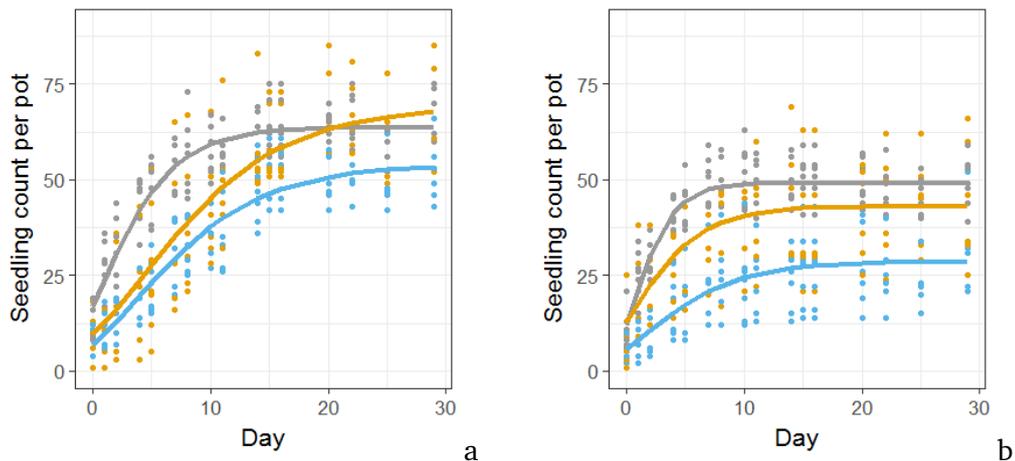
There was a significant effect of both organic matter ( $F_{2,30}=9.25$ ,  $P<0.001$ ) and water input ( $F_{1,30}=63.91$ ,  $P<0.001$ ) on the total number of *A. myosuroides* seeds germinating (see Supplementary Table S4.1) with fewest seeds germinating on high organic matter soil and the most on low organic matter soil. Increasing water input increased the

**Table 4.2.** Parameters and their standard errors of the Gompertz model (Equation 4.2) when fitted to germination data across Experiment 1 and to each treatment separately. In each case, the parameter  $A$  was fixed at zero.

Curve Parameter:	B		C		M	
	Estimate	SE	Estimate	SE	Estimate	SE
All data	0.2211	0.023	50.47	1.1	1.655	0.28
Low organic matter, low water input	0.5200	0.102	49.20	1.1	0.658	0.25
Low organic matter, high water input	0.2895	0.039	63.82	1.4	0.961	0.30
Medium organic matter, low water input	0.3032	0.064	43.12	1.4	0.637	0.45
Medium organic matter, high water input	0.1535	0.019	69.31	2.8	4.452	0.46
High organic matter, low water input	0.2275	0.063	28.74	1.7	2.063	0.75
High organic matter, high water input	0.1731	0.025	54.06	2.4	4.104	0.51

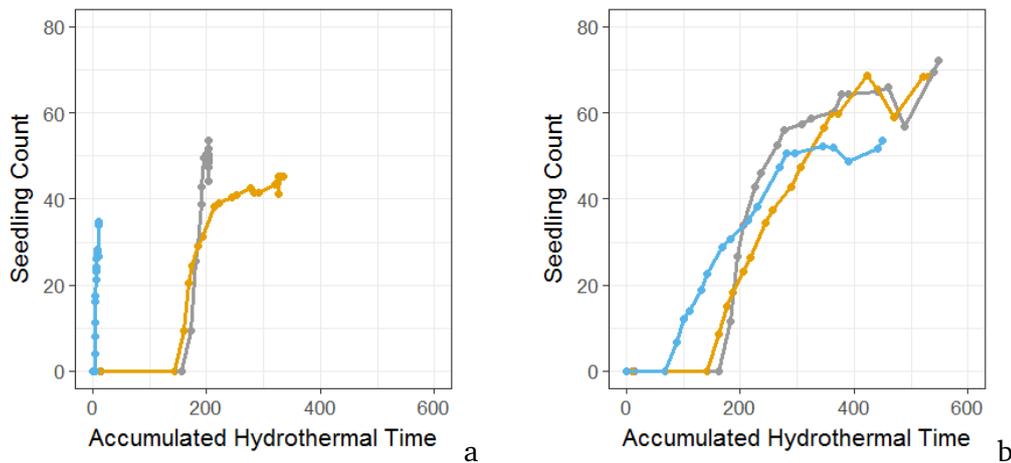
number of seeds germinating. There was no significant interaction between organic matter and water input on the total number of seeds germinating.

When we fit a single Gompertz curve (Equation 4.2) to the germination counts we account for 45.1% of the variance in the data set. By fitting a separate curve to each treatment we see a significant improvement ( $P < 0.001$ , see Supplementary Table S4.2) with this model accounting for 76.1% of the variance in the data set (Table 4.2). We see different shaped curves for each water input and different asymptotes for each organic matter indicating there is some interaction between the two (Figure 4.3).



**Figure 4.3.** Germination data with separate curves fitted for each level of organic matter and water treatment. (a) shows the data for low water input, (b) shows the data for high water input. Data points are shown as circles. The fitted curve is a solid line. Grey is low organic matter; Yellow is medium organic matter and blue is high organic matter.

When we fitted germination counts from Experiment 1 against hydrothermal time (Figure 4.4), the curves were much more similar in appearance across the three soil types indicating that the different levels of organic matter in each soil were allowing different levels of water retention and so accumulated hydrothermal time at different rates. At the low level of water input, the curves fitted for the low and medium organic matter were similar (Figure 4.4 a) with the germination counts and hydrothermal time not reaching as high a level as in the high watering treatment (Figure 4.4 b). However, on the high organic matter soil with low water input (Figure 4.4 a, blue line) the accumulation of hydrothermal time was particularly slow and germination seemed to exceed the expectation according to the accumulation of hydrothermal time. This may be because of the artificial nature of the soil used here. The calculations used to convert the theta probe measurements to water content were based on reference values for mineral soil and so the combination of a particularly dry watering regime with an artificial soil may have led to inaccurate estimates of the soil moisture in this case.



**Figure 4.4.** Germination data plotted against hydrothermal time with separate curves fitted for each level of organic matter. (a) shows the low water input, (b) shows the high water input. Data points are averages for each treatment. Grey is low organic matter; Yellow is medium organic matter and blue is high organic matter.

### Phenology

There was no significant effect (see Supplementary Table S4.3) of either soil organic matter or water input on the day of first flowering (Table 4.3).

**Table 4.3.** Summary of data for the day of first flowering. Means and their standard errors are shown for each treatment combination in Experiment 1.

	Mean (Julian day)	SEM
All data	123.1	0.821
Low organic matter, low water input	123.0	2.000
Low organic matter, high water input	125.0	3.367
Medium organic matter, low water input	122.6	1.571
Medium organic matter, high water input	124.0	2.082
High organic matter, low water input	121.0	1.528
High organic matter, high water input	123.0	12.292

### Plant Height

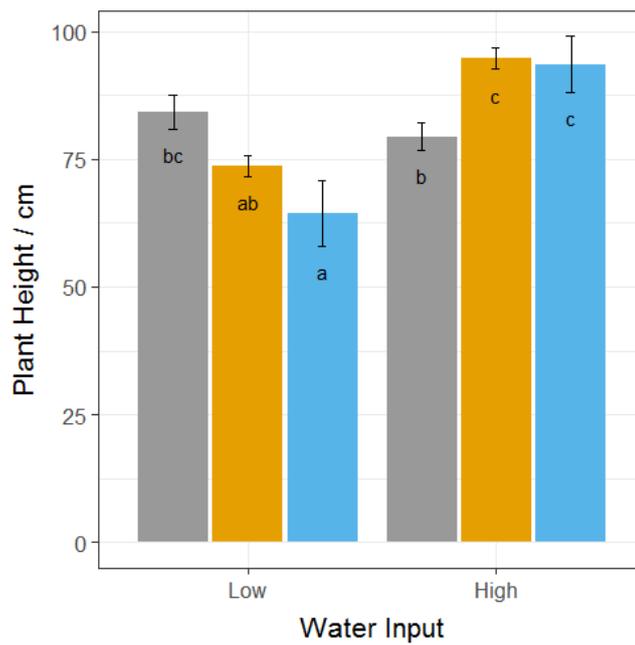
There was a significant effect of both water input ( $F_{1,30}=21.45$ ,  $P<0.001$ ) and its interaction with soil organic matter ( $F_{2,30}=9.74$ ,  $P<0.001$ ) on the height of the plant at maturity (see Supplementary Table S4.4). When water input is high the *A. myosuroides* plants were significantly taller than when water input was low. The interaction between soil organic matter and water input is particularly interesting because at low water input there is a tendency for plant height to decrease as organic matter increases whereas at high water input this trend is reversed and the shortest plants are found on the low organic matter soil (Figure 4.5).

### Seed Production

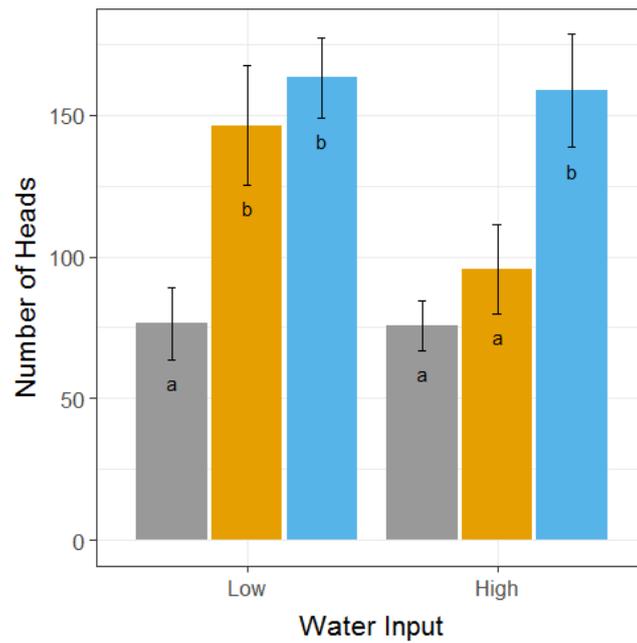
The total number of *A. myosuroides* seed heads was significantly affected by soil organic matter ( $F_{2,30}=15.54$ ,  $P<0.001$ , Figure 4.6) but not water input (see Supplementary Table S4.5). However, the dry weight of seed remained unaffected by soil organic matter or water input (see Supplementary Table S4.6).

### Biomass

Organic matter affected the dry weight of straw ( $F_{2,30}=32.15$ ,  $P<0.001$ , low organic matter = 12.9, medium organic matter = 23.6, high organic matter = 32.6). There was no effect of water input on the dry weight of straw (see Supplementary Table S4.7).



**Figure 4.5.** The height of *A. myosuroides* plants grown in trial one at two different levels of water input. Plants were grown on soil with three different levels of organic matter; low organic matter is shown in grey, medium organic matter shown in yellow and high organic matter shown in blue. The means of all pots are presented with error bars indicating  $\pm 1$  SEM. Bars labelled with the same letter are not significantly different from one another ( $P \leq 0.05$ ).



**Figure 4.6.** The number of seed heads per *A. myosuroides* plant grown in trial one at two different levels of water input. Plants were grown on soil with three different levels of organic matter; low organic matter is shown in grey, medium organic matter shown in yellow and high organic matter shown in blue. The means of all seven pots are presented with error bars indicating  $\pm 1$  SEM. Bars labelled with the same letter are not significantly different from one another ( $P=0.05$ ).

**Table 4.4.** Parameters and their standard errors of the Gompertz model (Equation 4.2) when fitted to germination data across Experiment 2 and to each pH treatment separately. In each case, the parameter A was fixed at zero.

Curve Parameter:	B		C		M	
	Estimate	SE	Estimate	SE	Estimate	SE
All data	0.3452	0.053	38.86	1.6	7.833	0.33
Low pH	0.3781	0.084	40.92	2.2	8.002	0.42
High pH	0.3243	0.073	36.72	2.4	7.730	0.50

Similarly, total plant biomass was significantly affected by organic matter ( $F_{2,30}=29.40$ ,  $P<0.001$ , low organic matter = 15.2, medium organic matter = 27.8, high organic matter = 36.6) but not water input (see Supplementary Table S4.8).

#### 4.4.2 Experiment 2: pH

##### Germination

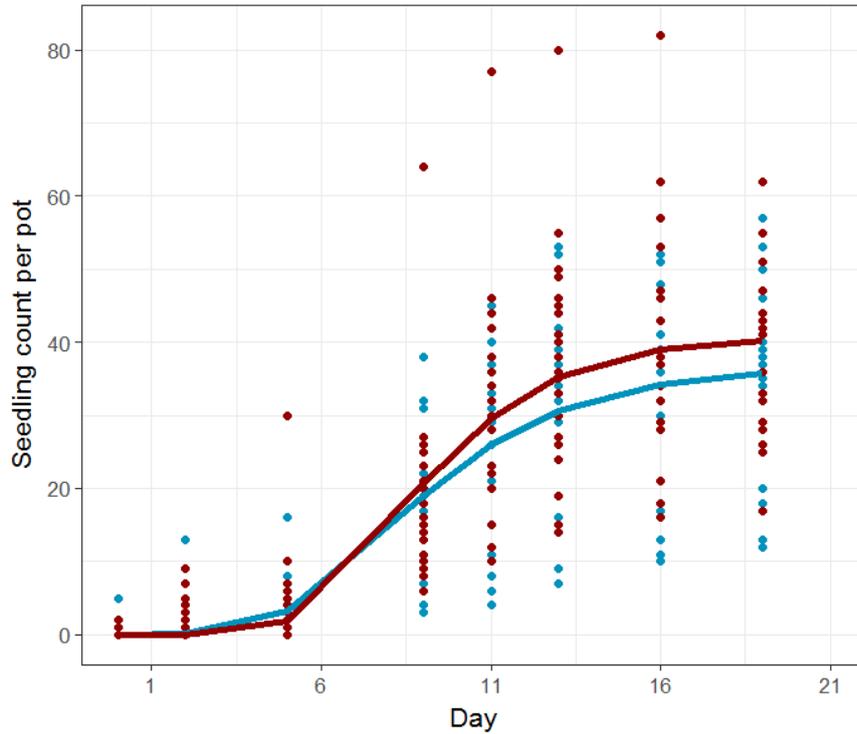
There was no significant effect of soil pH on the total number of seeds germinating (see Supplementary Table S4.9).

When we fit a single Gompertz curve (Equation 4.2) to the germination counts we account for 66.7% of the variance in the data set. By fitting a separate curve to each soil pH we see a marginal improvement ( $P=0.058$ , see Supplementary Table S4.10) with this model accounting for 67.1% of the variance in the data set (Table 4.4). These fitted curves indicate that a greater number of seeds germinate at lower pH (Figure 4.7).

#### 4.4.3 Experiment 3: pH and crop competition

##### Phenology

There was no significant effect of any treatment on the day of first flowering (Table 4.5, see Supplementary Table S4.11).



**Figure 4.7.** Germination data with separate curves fitted for each soil pH. Data points are shown as circles. The fitted curve is a solid line. Red symbolizes low pH and blue is higher pH.

**Table 4.5.** Summary of data for the day of first flowering in Experiment 2. Means and their standard errors are shown for each treatment combination.

	Mean (Julian day)	SEM
All data	168.1	1.630
Lower pH, <i>A. myosuroides</i> alone	166.1	5.347
Higher pH, <i>A. myosuroides</i> alone	167.7	6.058
Lower pH, <i>A. myosuroides</i> in competition	164.0	6.870
Higher pH, <i>A. myosuroides</i> in competition	162.4	9.458
Lower pH, wheat alone	171.9	0.404
Higher pH, wheat alone	169.6	0.782
Lower pH, wheat in competition	171.2	0.917
Higher pH, wheat in competition	170.2	0.600

**Table 4.6.** Summary of data for the height of the tallest tiller. Means and their standard errors are shown for each treatment combination.

	Low pH		High pH	
	Mean (cm)	SEM	Mean (cm)	SEM
<i>A. myosuroides</i> alone	79.0	7.97	69.7	5.30
<i>A. myosuroides</i> in competition	91.0	4.75	78.3	9.65
Wheat alone	79.5	1.59	76.6	1.19
Wheat in competition	78.0	1.64	75.0	0.71

### Plant Height

A small effect of pH ( $F_{1,31}=3.83$ ,  $P=0.060$ ) was observed on plant height (see Supplementary Table S4.12) with both *A. myosuroides* and wheat growing taller at lower pH, both when grown alone and in competition (Table 4.6). Interestingly, a much larger shade avoidance response (increased height in competition) was observed for *A. myosuroides* than the crop, which is constrained by the dwarfing genes bred into modern crop varieties.

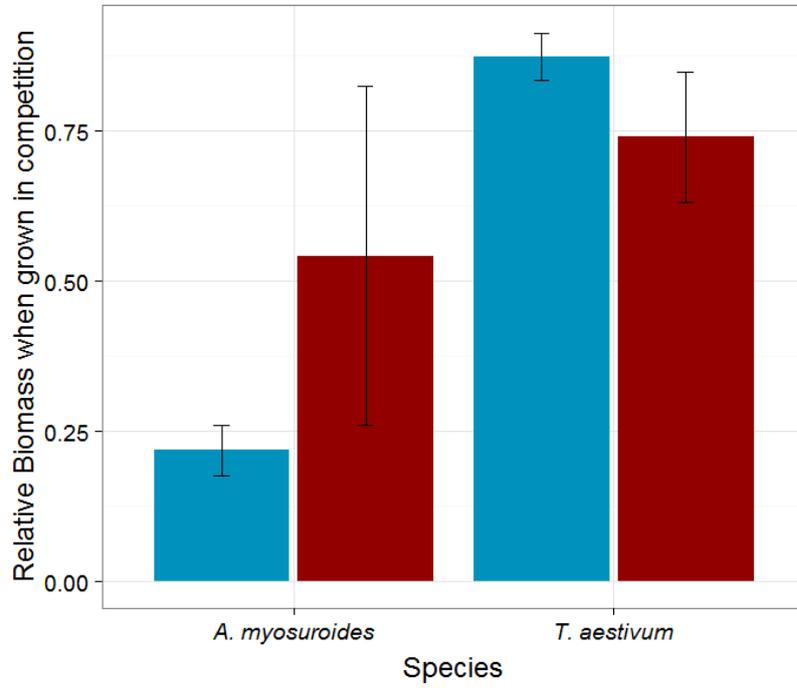
### Seed Production

There was a significant effect of competition ( $F_{1,34}=6.92$ ,  $P=0.013$ ) but not of pH on the number of seed heads produced (see Supplementary Table S4.13). However, there was no effect of any treatment on the dry weight of heads (see Supplementary Table S4.14).

### Biomass

The total plant biomass remained unaffected by pH or competition (see Supplementary Table S4.15). Interestingly when we consider the competitive performance of plants measured as relative biomass in competition compared to isolation there was some indication that the effect of pH interacts with species ( $F_{1,12}=3.37$ ,  $P=0.091$ , see Supplementary Table S4.16). Generally, the biomass of wheat was not reduced by competition to the same extent as occurs in *A. myosuroides*, but this competitive balance appears to be altered by pH (Figure 4.8). At higher pH, there was a relatively small reduction in

wheat biomass compared with the much greater reduction in *A. myosuroides* biomass. However, at lower pH, the differences in the relative reductions in biomass of the two species are smaller, with a smaller reduction in the *A. myosuroides* biomass and a greater reduction in wheat biomass relative to the responses recorded at the higher pH.



**Figure 4.8.** The relative biomass of wheat and *A. myosuroides* plants grown in competition compared to when grown in isolation. A value of one would indicate that there is an equal biomass produced when grown in competition as when grown in isolation. The means of seven pots are presented with error bars indicating  $\pm 1$  SEM. Data for lower pH are shown in red and for higher pH are shown in blue.

## 4.5 Discussion

As germination is a function of hydrothermal time (Bradford, 1995) we would expect it to change with water input. We would also expect increasing organic matter to improve the water retention capacity of the soil and so too to lead to an increased rate of germination. However, the results were somewhat contrary to this expectation. We did observe higher levels of germination when water input was high, yet the medium organic matter soil allowed more seeds to germinate than the high organic matter soil. We speculate this may be due to mulching from the compost used to elevate the soil organic matter. The change in germination with pH may also be due to the altered

chemistry of the soil affecting water uptake. These impacts of environmental properties on germination could have an impact in terms of management practices as delayed drilling is a common method of cultural control. However, if the timing of germination can be affected by environmental processes then perhaps this needs to be taken into consideration when developing management programs.

As plant height was affected by various soil properties this too could have important implications for management practices as the taller a plant is at maturity, the greater the opportunity for seed dispersal over longer distances meaning patches may expand in the following season (Howard *et al.*, 1991). However, this needs to be interpreted in the context of the trade-off between fewer, taller tillers and a greater number of shorter tillers with greater seed production.

The competitive balance between wheat and *A. myosuroides* was affected by soil pH with *A. myosuroides* having a greater relative growth at lower pH. This indicates that soil pH may have some influence on the location of *A. myosuroides* patches. It is likely this effect is related to the availability of nutrients at varying soil pH; for example, nitrogen, phosphorus, and potassium are all limited in availability in acid soil, whilst iron, zinc, and copper become limited in more alkaline soil (Brady, 1984). The contrasting rooting structure and function of *A. myosuroides* and wheat have been suggested as a possible reason for the current distribution of *A. myosuroides* in relation to variation in soil properties (Stratonovitch *et al.*, 2012).

When we compare these results to field observations obtained in a previous study (Metcalf *et al.*, 2016, Chapter 2) they support the conclusion that pH may have some controlling influence over the within-field distribution of *A. myosuroides*. In the field, we found higher densities of *A. myosuroides* at lower pH. If, as indicated here, more *A. myosuroides* seeds germinate on acidic soil and it is better able to compete with wheat then this could explain the higher densities of *A. myosuroides* observed on more acidic soil.

Some of the responses to increased organic matter observed here may not have been due to the changes in soil function, but rather due to the increased fertility owing to the compost addition. On farm, an increase in soil organic matter could also lead to increased fertility and so it is not always possible to separate these effects. However, if a farmer is selectively applying fertiliser to parts of the field to account for this then

it may be necessary to investigate the effects of organic matter further, independently of soil fertility, through the addition of inorganic nutrients to the low organic matter treatments. This would then allow the study of changing soil function with organic matter and its effects on the life-cycle of the weed, independently from the effects of increased fertility.

These results raise some interesting questions in terms of management of *A. myosuroides* and whether management options should be tailored to within-field environmental gradients. We have presented evidence that high organic matter soil is favourable to *A. myosuroides* seed production, but perhaps less so for germination. We have also found further evidence that there is a subtle difference in the optimum pH for wheat and *A. myosuroides*. Combining our experience in field and pot experiments, we suggest soil above a pH of 6, is less favourable to *A. myosuroides* but still optimal for wheat. However further research would be needed to understand how the system responds to a wider range of soil organic matter contents, watering, and pH.

These results indicate a potential trade-off between increasing organic matter in the soil for crop growth and reducing it for *A. myosuroides* control as the number of seed heads can be significantly reduced by lowering soil organic matter. This raises questions about the suitability of popular management techniques such as minimum tillage in a high *A. myosuroides* situation. Potential management options for further exploration could be the use of liming where pH is particularly low as part of a suite of measures (including improving soil structure and drainage) designed to manipulate habitat suitability for *A. myosuroides*. The use of competitive crop cultivars could also be investigated to determine if cultivars can remain competitive on low soil pH or high organic matter and so would be better able to suppress *A. myosuroides* growth under these conditions.

## 4.6 Conclusions

We have shown that soil organic matter, moisture, and pH can affect various aspects of the life-cycle of *A. myosuroides*. The influence of each of these soil properties is varied but each may contribute to the determinants of patch locations in the field. These effects of soil properties on the life-cycle may present opportunities for tailoring management

to site conditions or even within-field environmental gradients.

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## Chapter 5

# The Implications of Spatially Variable Pre-Emergence Herbicide Efficacy for Weed Management

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In addition to my experiments on the direct and indirect effects the soil has on the life-cycle of *A. myosuroides* (Chapter 4), I investigated how the soil can mediate the efficacy of control measures implemented by the farmer. My third hypothesis that soil organic matter affects the efficacy of flufenacet and pendimethalin against *A. myosuroides* and the ability of the weed to withstand sub-lethal doses of those herbicides, addresses the idea that changes in control levels due to soil properties may influence the within-field distribution of *A. myosuroides* in similar ways to the direct influence of the soil on the *A. myosuroides* life-cycle.

Initially, I did a preliminary investigation to see if pre-emergence control could be influenced by changing soil organic matter and water input. This preliminary study is detailed below in Sections 5.i and 5.ii.

Following on from the preliminary investigation I went on to look at some of the most interesting results in more detail by focussing on the effect of soil organic matter. I considered a full dose-response to flufenacet and pendimethalin on soil with varying levels of organic matter. I also grew the plants on to maturity in order to look at the sub-lethal effects of the herbicides and how these varied depending on the amount of organic matter in the soil. In addition to these experiments I analysed the data further by using it to parameterise a crop competition model to see if the difference in control and sub-lethal effects observed on the different soils would lead to a substantial reduction in seed return under competition. This work is detailed in Sections 5.1–5.7 and is under revision following review with Pest Management Science.

## 5.i Preliminary Methods

I studied the effect of changing soil organic matter (3 levels) and water input (2 levels) on the efficacy of flufenacet and pendimethalin (no herbicide, low, and high doses) against *Alopecurus myosuroides* Huds. (black-grass) seedling survival and growth in winter 2014–15. The experimental design was a randomized complete block design with 10 replicates of each treatment combination. I assigned an extra 6 replicates to each treatment that received no herbicide as additional controls. I germinated *A. myosuroides* seeds from the Broadbalk experiment in Petri dishes in a Sanyo MLR-350 environmental test chamber providing a 17°C 14-hour day, 11°C 10-hour night for seven days. I transplanted eight seedlings into each 10-cm diameter pot on 9th December 2014. The following day I sprayed the pots with the required dose of herbicide per the treatment structure outlined below. I placed the pots in an unheated glasshouse and allowed the plants to grow for eight weeks prior to assessment (2nd February 2015).

### Soils

I created three soils with varying organic matters, whilst maintaining other soil properties at relatively constant values by mixing sand, loam, and composted bark in different ratios as described for Experiment 1 in Chapter 4.

**Table 5.i.** Application rates of two pre-emergence herbicides in the preliminary investigation.

Dose	Flufenacet (g a.i./ha)	Pendimethalin (g a.i./ha)
None	0	0
Low	7.5	200
High	60	1000

### Water Input

I established two watering regimes with half of the pots receiving just enough water to prevent any signs of wilting (water limited). The other half received twice this amount of water (sufficient water).

### Herbicides

For each herbicide, I chose a low dose known to achieve poor efficacy under glasshouse conditions and a high dose known to achieve good efficacy under glasshouse conditions (Table 5.i).

### Assessment

I assessed survival as the proportion of individuals that remained alive eight weeks after the application of the herbicide.

### Data Analysis

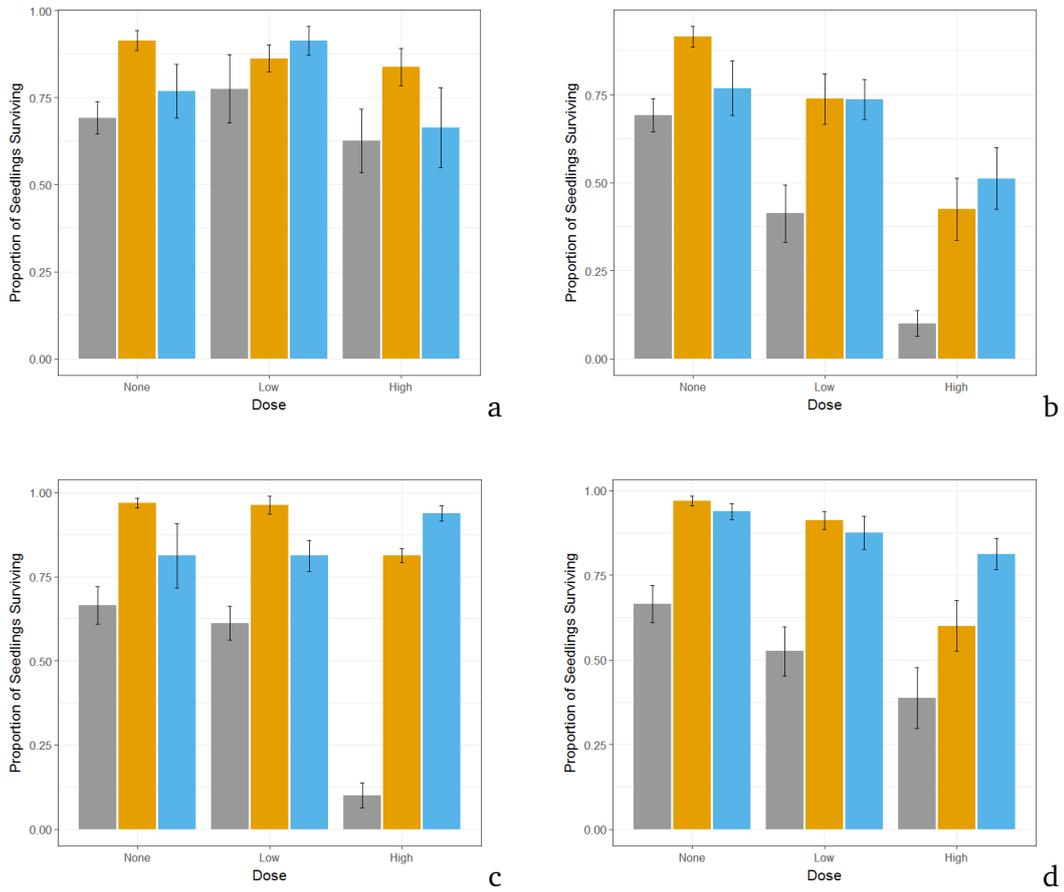
I analysed the data in GenStat (Payne, 2013) using a generalized linear model to determine statistically significant differences between treatments. As the data are proportions I assumed they followed a binomial distribution and so used a logit link function.

## 5.ii Preliminary Results

The proportion of seedlings surviving eight weeks after spraying was significantly affected by both soil organic matter and water input (Figure 5.i). Survival without herbicide was generally greatest on the medium organic matter soil. However, at high water input in the presence of high doses of either herbicide, survival on the high organic matter soil was greater (Figure 5.i c and 5.i d). For flufenacet, the herbicide efficacy was generally poor at the chosen doses (Figure 5.i a and 5.i c) and effective control of *A. myosuroides* was only observed at the high dose on the low organic matter soil when water input was high. Pendimethalin had a greater efficacy across all treatments (Figure 5.i b and 5.i d) but again, the greatest reduction in survival was seen on the low organic matter soil.

These results indicate that the efficacy of pre-emergence herbicides is affected by soil conditions. Based on these preliminary data I decided that the change in herbicide efficacy in response to organic matter was of the most interest. I continued with the use of two pre-emergence herbicides but did not include different levels of watering. I also decided that it would be interesting to consider a full dose-response to ensure I covered a range of efficacies. I wanted to incorporate higher doses up to field rate and above, as I saw little effect of the low doses used here and even at the high doses (which corresponded to only 25% of field rate for flufenacet and 83% of field rate for pendimethalin) the reduction in survival was small. As well as investigating survival rate following the application of pre-emergence herbicides, this full study looks at sub-lethal effects; addressing the second part of my hypothesis that soil organic matter affects the ability of *A. myosuroides* to withstand sub-lethal doses of pre-emergence herbicides. The following is under revision following review with Pest Management Science.

Although I did not go on to further investigate the effect of water input, these preliminary results indicate that water input does interact with soil organic matter to impact on control. This supports the findings of Blair *et al.* (1994), Orson *et al.* (1998) and Collings *et al.* (2003) that water stress and weather play important roles in the efficacy of pre-emergence herbicides. Further studies could provide useful insights into the interaction between stable soil variables such as organic matter and dynamic weather factors such as rainfall on the efficacy of pre-emergence herbicides.



**Figure 5.i.** Proportion of seedlings surviving eight weeks after the application of pre-emergence herbicides. Means  $\pm$  SEM are shown for each dose tested. In each panel, the low organic matter is shown in grey, medium organic matter in yellow and high organic matter in blue. Watering treatments and herbicides are shown in separate panels, (a) Flufenacet, low water input, (b) Pendimethalin, low water input, (c) Flufenacet, high water input (d) Pendimethalin, high water input.

## 5.1 Summary

The efficacy of pre-emergence herbicides within fields is known to be spatially variable because of heterogeneous soil properties, partly explaining why weed distribution is patchy. Here we quantified this variability for two widely used pre-emergence herbicides, flufenacet and pendimethalin, in controlling *A. myosuroides*, on soil with varying levels of soil organic matter using pot experiments. The implications of this variability for weed management was then investigated using a crop / weed competition simulation model that predicted the combined effects of the observed variable weed mortality and sub-lethal effects on weed seed production.

The level of soil organic matter played a critical role in determining the level of control achieved: in the pot experiments, the two high organic matter treatments consistently had more surviving weed plants with higher biomass than the low organic matter soil. Where there were survivors, even when high doses of herbicide were applied, the plants had the ability to recover to produce the same amount of seed as if no herbicide were applied, in the absence of competition. The competition model predicted that weeds surviving pre-emergence herbicides were able to compensate for sub-lethal effects even when competing with a crop. As a result, the ED50 was consistently higher for weed seed production than either seedling mortality or biomass and this difference was greatest on high organic matter soil.

These results could have important implications for the precision management of *A. myosuroides* as our improved understanding of the variation in levels of control achieved by pre-emergence herbicides on soil with contrasting organic matter would allow adjustment of the application rate of the herbicide to account for within-field gradients of soil organic matter. However, the results from the modelling also emphasised the importance of crop competition in limiting the capacity of weeds surviving pre-emergence herbicides to compensate and replenish the seedbank, particularly where there is resistance to contact herbicides. This new knowledge needs to be integrated within the wider context of the impact of variable soil on weed growth and competition across the whole weed life-cycle.

## 5.2 Introduction

Herbicides are an important component of weed control programmes and soil-applied herbicides are particularly important for controlling germinating weeds in the context of the rapid evolution of resistance to contact herbicides. Generally, these pre-emergence herbicides are applied uniformly across the field at doses recommended by the manufacturer. These recommended doses are given irrespective of variation in soil properties and for many pre-emergence herbicides the only advice, with regards to soil, is that they should only be used on soil with organic matter up to 10%. In Great Britain, this is seldom problematic, given that the average amount of soil organic matter (0–15 cm) in arable and horticultural land is 3.07% (Emmett *et al.*, 2010).

*Alopecurus myosuroides* Huds. (black-grass) is a particularly problematic weed of winter wheat (*Triticum aestivum* L.) in the UK and so its control is of concern. Given increasing problems of evolving resistance to contact herbicides (Moss *et al.*, 2007), and the decreasing number of options available for chemical control, the currently available pre-emergence herbicides (based largely on flufenacet and pendimethalin) are an important tool in the arsenal against this pernicious weed. *Alopecurus myosuroides* exhibits patchy distributions within fields, yet its control is often through uniform application of herbicides. As with many species, it is thought that these patchy distributions in arable fields are strongly affected by their environment, in particular, the soil (Radosevich *et al.*, 2007; Metcalfe *et al.*, 2016 (Chapter 2)).

Soil properties not only affect the life-cycle of the weeds of weeds directly (Metcalfe *et al.*, 2017 (Chapter 4)) but they can also have an indirect effect by altering the efficacy of some herbicides (Pedersen *et al.*, 1995). Organic matter in the soil can lead to adsorption of herbicide (Farenhorst, 2006). Different herbicides may be more, or less, adsorbed by organic matter, dependent on their physical and chemical properties (Nordmeyer, 2015) with flufenacet and pendimethalin both adsorbing highly to the soil (pendimethalin  $K_d$ : 2.23 to 168 (Shaner, 2012) and flufenacet  $K_d$  = 0.77 to 4.52 (Gajbhiye & Gupta, 2001). If the amount of soil organic matter varies across the field, there may be parts of the field where these pre-emergence herbicides are less available to the plant. This, in turn, may lead to differential control across the field and so increases the chance of the establishment of weed patches where herbicide control is reduced.

As pre-emergence herbicides are applied directly to the soil, it is particularly impor-

tant to understand how varying soil properties within fields may affect their efficacy. Some studies have considered this and shown that organic matter influences herbicide efficacy. For example, Nordmeyer (2015) showed that a relatively small increase in organic matter from 2.2 to 3.5% can impact the efficacy of chlortoluron against *A. myosuroides*. Blumhorst *et al.* (1990) also demonstrated a strong correlation between soil properties and the herbicidal activity of five different herbicides against *Abutilon theophrasti* Medik. (velvetleaf) and *Setaria viridis* L. (green foxtail). Despite this previous research indicating that varying organic matter in the soil can lead to reduced weed control, little has been done to understand the response of two key pre-emergence herbicides in the control of *A. myosuroides* to such changes in soil organic matter and the implications for weed management in terms of potential weed seed return.

Given that in a field with spatially heterogeneous organic matter we would expect different levels of control, it is also important to consider any sub-lethal effects on the survivors and their impact through the rest of the growing season. When implementing weed control strategies, the focus is often on diminishing seed return. Modelling is frequently used to investigate the effects of different management practices (e.g. cultivation (Cousens & Moss, 1990; Grundy *et al.*, 1999), crop rotations (Garrison *et al.*, 2014), patch spraying (Paice *et al.*, 1998)). Where these models include the use of herbicide, however, they generally model the effect of herbicide simply as a proportional kill of weed seedlings with the implicit assumption that the survivors remain unaffected (Holst *et al.*, 2007). Sub-lethal effects have been shown to be important in many species, for example, Rotchés-Ribalta *et al.* (2015) showed that some species show no decrease in biomass at harvest irrespective of the dose of herbicide received and Riemens *et al.* (2009) showed that with increasing dose the number of seeds per gram of fresh weight can decrease. Often when field data are collected on herbicide efficacy there is a marked difference between the level of control achieved at the seedling stage and the head stage (e.g. Moss *et al.*, 2016). It cannot, therefore, be assumed that pre-emergence efficacy at the seedling stage is equivalent to a proportional decrease in seed return in the absence of subsequent herbicide activity. Variability in pre-emergence herbicide activity needs to be understood in the context of the effect of soil heterogeneity on the rest of the weed life-cycle.

Our aim was to quantify the effect of variable soil organic matter on the seed return of *A. myosuroides* following the application of flufenacet or pendimethalin at a range

of doses. We examined both the level of control achieved by those two herbicides on soil with different amounts of organic matter as well as sub-lethal effects of the herbicide, and the ability of plants to recover and produce viable seed in the context of crop competition. To investigate this, we considered three different levels of organic matter, typical of arable fields in the UK, and a range of herbicide dose rates applied to *A. myosuroides* seedlings in pots. We hypothesized that increasing organic matter would lead to decreased efficacy of both herbicides in the control of *A. myosuroides* and that sub-lethal doses would lead to fitness costs causing reduced growth and fecundity (the fitness cost also being determined by soil properties). We used regression analyses to determine whether soil organic matter impacts the shape of the dose-response curves for these two herbicides observed in pots and used the results from the pot experiment to parameterise a simulation model of crop / weed competition and weed seed production in the field. An increased understanding of how local soil conditions affect the efficacy of pre-emergence herbicides and the implications for *A. myosuroides* population dynamics will increase our ability to properly manage this prolific agricultural weed, particularly in the context of precision weed control and integrated weed management strategies.

## 5.3 Methods

### 5.3.1 Soils

To isolate the effects of soil organic matter from the many covarying soil properties we created three artificial soils with varying amounts of organic matter, whilst maintaining other soil properties at relatively constant values by mixing sand, loam, and composted bark in different ratios (Table 5.1). Composted bark is homogeneous in its organic matter content and so allowed fine adjustment of soil organic matter whilst adding minimal additional nutrients. Samples of each soil mixture were tested by the laboratories at SOYL (Newbury UK) using loss on ignition to establish the amount of organic matter (Table 5.1) The range of organic matters achieved was typical of UK arable land. We created two soils with organic matter less than 3% (typical of British arable soil) and one soil representing particularly high levels but still within the 10% level quoted on many herbicide labels. Each soil type was used to fill 180 10-cm diameter pots and 90 25-cm diameter pots giving a total of 540 10-cm diameter pots and 270 25-cm diameter pots.

**Table 5.1.** The volumetric composition of the three soil mixtures used, their percentage organic matter measured by loss on ignition, and the measured pH of the soils.

Soil mixture	Coarse sand (% by volume)	Fine sand (% by volume)	Loam (% by volume)	Composted bark (% by volume)	OM (LOI % w/w)	pH
Low organic matter	35	35	22.5	7.5	1.93	7.16
Medium organic matter	20	20	45	15	2.37	7.00
High organic matter	0	0	75	25	6.15	7.00

### 5.3.2 Plant Material

We used *A. myosuroides* seed from a plot on the Broadbalk long-term experiment established at Rothamsted Research (Harpenden, UK) in 1843 that had never received any herbicides (Moss *et al.*, 2004). This population has been shown to be free of any evolved herbicide resistance. The seed was collected in 2014 and had been stored in darkness from harvest until the start of this experiment. We germinated *A. myosuroides* seeds in Petri dishes in a Sanyo MLR-350 environmental test chamber providing a 17°C 14-hour day, 11°C 10-hour night for seven days. Seeds were germinated in Petri dishes lined with three Whatman No.1 90 mm diameter qualitative filter papers and 5 ml of  $\text{KNO}_3$  ( $2 \text{ g l}^{-1}$ ). We transplanted eight germinated seeds (radicle just emerged) into each 10-cm diameter pot on 23rd February 2016. We placed the pots in an unheated glasshouse and allowed the plants to grow for six weeks prior to assessment. All plants received water as required.

### 5.3.3 Pre-emergence Herbicides

Flufenacet (Bayer CropScience Ltd) and pendimethalin (BASF plc) are two active ingredients present in pre-emergence herbicide products and are widely used in UK cereals. They are registered in several countries for the control of most annual grasses and common weeds in cereals, fruit, and vegetables. Here we tested their efficacy against *A. myosuroides*. Pendimethalin is a residual dinitroaniline herbicide (HRAC: K1) and flufenacet is an oxyacetamide herbicide (HRAC: K3). We applied each herbicidal active ingredient separately pre-emergence, (one day post sowing before any shoots had emerged) using a laboratory track sprayer delivering  $222 \text{ L ha}^{-1}$  at 210 kPa through a Teejet 110015VK ceramic nozzle, 50 cm above the soil surface. We applied a full range of doses with rates of 0, 1/64, 1/32, 1/16, 1/8, 1/4, 1/2, 1x and 2x recommended field rates (UK) of 240 and  $1200 \text{ g a.i. ha}^{-1}$  for flufenacet and pendimethalin, respectively. For each herbicide each dose was applied to 10 pots of each soil type. The experimental design was a randomized complete block design with 10 replicates of each treatment combination (each herbicide at each dose on each soil, 540 pots in total).

### 5.3.4 Herbicide Efficacy

Six weeks after the application of the pre-emergence herbicides we assessed survival as the proportion of individuals that remained alive in each pot. We assessed the average size of surviving plants by counting the number of tillers present in each pot and dividing that by the number of survivors to give an indication of the growth stage of the plants. We measured biomass on five randomly selected replicates by cutting all plant material at the ground level and taking a total dry weight per pot.

### 5.3.5 Sub-lethal Effects

To consider the sub-lethal effects of flufenacet and pendimethalin and how these are affected by soil organic matter as the plant matures we kept five replicates of each soil-herbicide-dose combination. These were not destructively assessed for biomass. Where there were survivors, we selected the median sized plant from each pot and transplanted it into a 25-cm diameter pot containing the same soil mixture. These plants were grown outside under netting. The same randomization as in the glasshouse was maintained. Plants were watered as required. No additional inputs were added to the soil; however, fungicides and insecticides were applied as required.

We recorded the Julian day of first flowering for each of these plants. Once all plants had flowered, we measured the height of the tallest tiller and the number of seed heads produced (27th July 2016). On the 24th August 2016, we cut all biomass at ground level and measured the total dry straw biomass. To assess the effect of soil organic matter on fecundity we measured the total fresh weight of the seed heads and calculated total dry weight from a subsample of seed. We also measured the viability of the produced seed by germination assay: following three months' storage in darkness at 18°C and 35% humidity, we assessed the viability of the seed produced by assessing germination in Petri dishes. We set up three Petri dishes for each sample with three Whatman No.1 90 mm diameter qualitative filter papers per dish. We put 50 seeds, representative of the uncleaned sample, and 5 ml of KNO<sub>3</sub> (2 g l<sup>-1</sup>, Riedel-deHaen analytical grade) into each dish and then incubated the dishes in a Sanyo MLR-350 environmental test chamber delivering 17°C 14-hour day, 11°C 10-hour night for 14 days. Following incubation, we counted the number of seeds that had germinated (visible radicle).

### 5.3.6 Data Analysis

We used the *drc* package in R (Ritz *et al.*, 2015) to find the best model to describe the dose-response relationships investigated in our experiments (ignoring treatment structure). We chose from log-logistic (3, 4, and 5 parameters), Weibull (type 1 and 2, with 3 and 4 parameters) and Cedergreen-Ritz-Streibig (4 parameters; A, B, and C types, in all types the lower limit is fixed to 0) (Table 5.2), as well as linear, quadratic and cubic models to capture any departures from these typical dose-response functions. Using the chosen best-fit model for a given data set, we assessed the significance of each treatment. First, we allowed the parameters of the model to depend on herbicide to test the hypothesis that the dose-response curves for flufenacet and pendimethalin were different from one another. We then allowed the parameters of the model to depend on soil type to test the hypothesis that the amount of organic matter in the soil affects the dose-response. If allowing the parameters to depend on both herbicide and soil type significantly improved the model ( $P \leq 0.05$ ), we then assessed the significance of including an interaction term. For the resulting best fit model, we checked each parameter for its importance by setting it to a common value across treatments and testing if the residual sum of squares was significantly altered. If not, the parameter was fixed and the next parameter assessed. We assessed parameters sequentially, beginning with the asymptotes before considering any gradient and timing parameters.

### 5.3.7 Modelling

In our experiments, the potential for seedlings surviving sub-lethal effects of pre-emergence herbicides to mature and produce fresh seed was quantified. However, the experiment did not include competition with the crop to avoid confounding the effects of soil organic matter on competitive ability and the ability to recover from sub-lethal doses. However, without including competition the experiment did not fully capture the potential fitness penalty of reduced seedling size and the capacity of weeds to compensate for sub-lethal herbicide effects when competing with a crop. Given that inter-specific competition is asymmetric, we would hypothesise that survivors will be disproportionately impacted by competition from the crop and this effect would increase disproportionately with greater herbicide efficacy. To challenge this hypothesis, we combined data from the pot experiment with a simulation model of crop–weed

**Table 5.2.** The models considered for describing the dose-response relationships.

Model	Expression	Parameterisation
Log-logistic	$f(x) = c + \frac{d - c}{(1 + \exp(b(\log(x) - \log(\eta)))^\gamma)}$	5 parameters
		4 parameters, $\gamma = 1$
		3 parameters, $c = 0$
Cedergreen-Ritz-Streibig	$f(x) = \frac{d + \gamma \exp(-1/x^\alpha)}{1 + \exp(b(\log(x) - \log(\eta)))}$	A type, $\alpha = 1$
		B type, $\alpha = 0.5$
		C type, $\alpha = 0.25$
Weibull type 1	$f(x) = c + (d - c) \exp(-\exp(b(\log(x) - \log(\eta))))$	4 parameters
		3 parameters, $c = 0$
Weibull type 2	$f(x) = c + (d - c)(1 - \exp(-\exp(b(\log(x) - \log(\eta))))))$	4 parameters
		3 parameters, $c = 0$

competition that has been parameterised and validated for *A. myosuroides* in winter wheat (Storkey & Cussans, 2007). The model is weather driven and operates on a daily time step. Before the onset of competition at canopy closure, weed growth is modelled as an exponential function of effective day degrees (Storkey *et al.*, 2003) after which competition for resources are modelled using functions developed in the INTERCOM model (Kropff & Spitters, 1992). Weed seed production is calculated from the allometric relationship with mature weed biomass.

The model was initialised with a weed seedbank density of 5000 seeds  $\text{m}^{-2}$ , 20% of which were in the upper soil layer, from which all seeds are available for germination, the remaining seeds have a smaller chance of germination according to a linear relationship with soil depth. Wheat density was set to 300 plants  $\text{m}^{-2}$ . Crop and weed emergence was set to 31st September—typical of agronomic practice for the UK. The number of emerged weed seedlings was calculated using a proportion sampled from a distribution function parameterised from a series of field experiments (Stratonovitch *et al.*, 2012). A proportion of these seedlings were killed using the mortality figure given by the best model fit for each treatment combination observed in the pot experiments. The mature biomass and seed production of the surviving weed plants was simulated using ten years of weather data measured at Rothamsted Research (Hertfordshire, UK) between 2006 and 2015 so capturing seasonal variability in the competitive balance between the crop and weed (Storkey & Cussans, 2007). For each year, the model was run 100 times using a new value for proportional germination sampled from the Weibull probability distribution (skewed towards lower emergence) to introduce stochasticity to do with variability in establishment.

The model was used to run two scenarios for each soil-herbicide-dose combination included in the pot experiments: (i) with crop competition, and (ii) without crop competition. Sub-lethal effects were included in the simulation by reducing weed seedling biomass and green area at the end of the exponential growth phase by the proportion predicted using the dose-response model that fitted the data from the pot experiments best. The output seed production from the simulation model was then analysed in the same way as the data from the experiments and a dose-response curve fitted to see if the different levels of survival and sub-lethal effects experienced on different soil and following the application of different herbicides at a range of doses can affect the resulting seed production.

**Table 5.3.** Fitted parameter values for the Cedergreen-Ritz-Streibig model used to describe the dose-response of the proportion of *A. myosuroides* seedlings surviving six weeks after the application of two pre-emergence herbicides on three levels of soil organic matter. Common parameters were fitted for both herbicides.

Parameter	Estimate	Standard error
$b$	1.777	0.2258
$d$	0.773	0.0451
$\eta$ – low organic matter	0.097	0.0170
$\eta$ – medium organic matter	0.234	0.0500
$\eta$ – high organic matter	0.374	0.0850
$\gamma$	1.187	0.5743

## 5.4 Results

A Cedergreen-Ritz-Streibig model (type C) best described the survival data. The fit of the model was significantly improved by incorporating soil organic matter but there was no improvement in the model when two separate curves were fitted for each active ingredient. In the model incorporating soil organic matter, parameters  $b$ ,  $d$  and  $\gamma$  could be fixed to be common for all soil types. However, fixing the  $\eta$  parameter caused a significant change in the model and so this was allowed to depend on soil organic matter (Table 5.3). There is not a direct biological correspondence for the  $\eta$  parameter in the Cedergree-Ritz-Streigbig model but it does provide a lower bound on the ED50 level and so relates to the placement of the curve on the dose axis. This type of model accounts for hormesis: there were more survivors at low doses of herbicide than in the controls that received no herbicide (Figure 5.1).

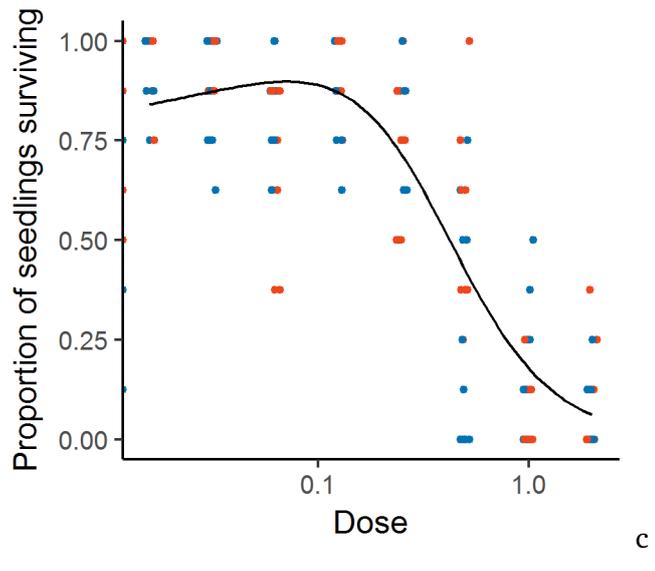
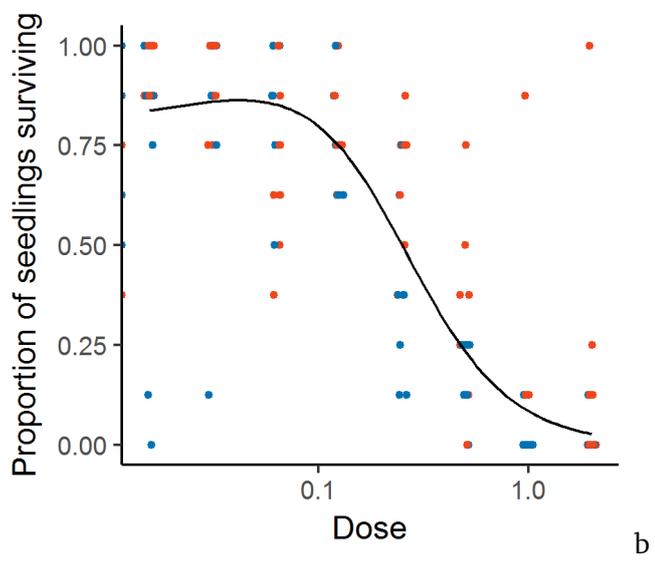
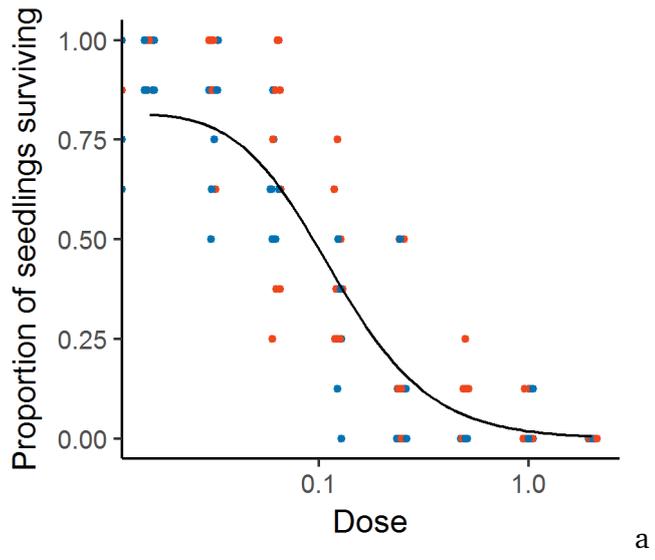


Figure 5.1. Figure legend on page 125.

**Figure 5.1.** (Figure on page 124.) The proportion of seedlings surviving six weeks after the application of two pre-emergence herbicides on soil with varying levels of organic matter: (a) low, (b) medium, and (c) high. Points indicate the response of each sample (flufenacet in blue, pendimethalin in red) and the fitted model is shown by a solid black line (Fitting separate lines to each soil type significantly improved the fit of the model but there was no significant difference between the two herbicides so a single line was fitted across both). Dose is given as a proportion of recommended field rate.

The relative growth stage, as indicated by the number of tillers, at six weeks after spraying showed a 3-parameter log-logistic response to the dose of herbicide applied. The fit of this model was significantly improved by fitting separate curves to each soil organic matter and herbicide and so their interaction was also assessed. Allowing an interaction between the two herbicides and soil organic matter also significantly improved the fit of the model. All parameters except  $\eta$  could be fixed to be common across treatments without significantly reducing the goodness of fit (Supplementary Table S5.1). The plants grown in the lowest organic matter soil showed a reduction in the number of tillers at lower doses of herbicide than was observed for medium or high levels of soil organic matter. Flufenacet reduced the number of tillers by 50% at lower doses than was seen for pendimethalin (Supplementary Table S5.1,  $\eta$  represents ED50 value) but this difference was less marked on high organic matter soil (Supplementary Figure S5.1).

The size of the seedlings as indicated by dry biomass measurements (natural logarithms) showed a 4-parameter log-logistic response to dose. Allowing separate curves to be fitted for each soil type and each herbicide significantly improved the model ( $P < 0.05$ ) so we tested for an interaction between them. This again significantly improved the fit of the model. The  $b$ ,  $c$  and  $d$  parameters of the logistic curve could be fixed to be common across all soil types and both herbicides, leaving only the  $\eta$  parameter to vary (Table 5.4). For the logistic curve, the  $\eta$  parameter signifies the ED50 value indicating that the positioning of the curves on the dose axis is affected by soil and herbicide. For both herbicides, the ED50 is lowest on low organic matter soil and increases with organic matter. For pendimethalin the ED50 is higher than it is for flufenacet, across all soil types. However, this difference is less marked on the highest organic matter soil (Figure 5.2).

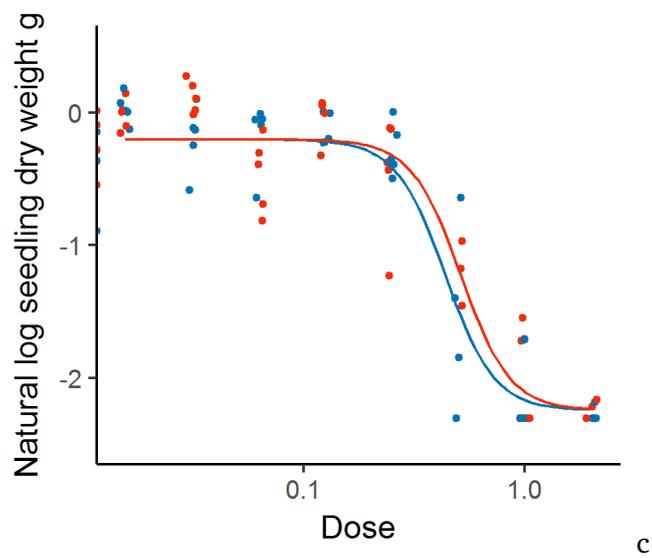
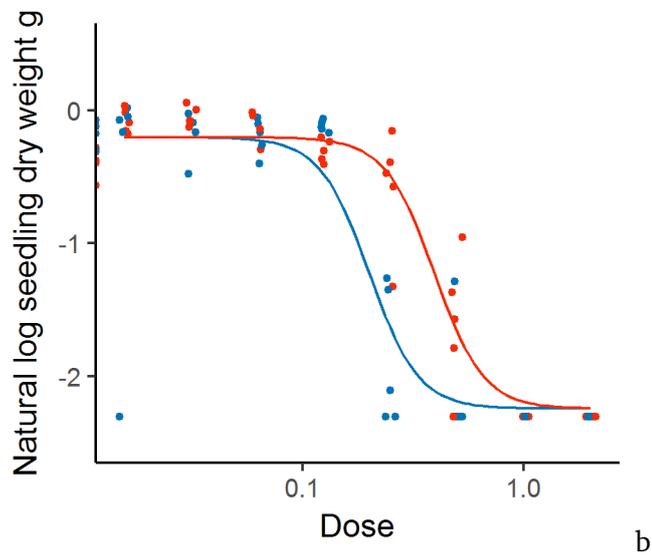
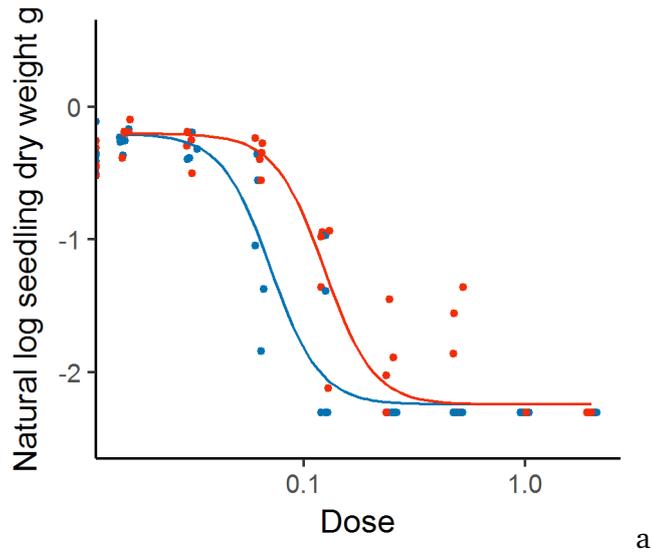


Figure 5.2. Figure legend on page 127.

**Figure 5.2.** (Figure on page 126.) The log dry weight of seedlings surviving six weeks after the application of two pre-emergence herbicides on soil with varying levels of organic matter: (a) low, (b) medium and (c) high. Points indicate the response of each sample) and the fitted model is shown by a solid line (flufenacet in blue, pendimethalin in red). Dose is given as a proportion of recommended field rate.

Despite significant effects of the herbicide used, the dose applied, and the amount of soil organic matter on plant numbers, growth stage, and size at six weeks, these effects were diminished as the plants were grown on to maturity. There were few survivors at the higher doses used, particularly on the low organic matter treatment, and so there was less replication in this part of the experiment looking at sub-lethal effects. There was no significant change in the Julian day of flowering ( $P \leq 0.05$ ) with herbicide or dose, nor a response to soil organic matter.

The number of seed heads and the dry weight of seed produced by each plant was conserved across the full range of doses and there was no significant effect of dose or herbicide in any model. However, a significant response to soil organic matter was detected ( $P < 0.001$ , ANOVA) with the number of heads per plant increasing with organic matter (Table 5.5). It is likely that this is a result of a “fertilising” effect of the additional organic matter on weed growth.

The total dry weight of the mature plants was, however, affected by dose as well

**Table 5.4.** Fitted parameter values for the log-logistic model used to describe the dose-response of the log dry biomass of *A. myosuroides* seedlings surviving six weeks after the application of two pre-emergence herbicides on three levels of soil organic matter.

Parameter	Estimate	Standard error
<i>b</i>	3.895	0.5442
<i>c</i>	-2.242	0.0402
<i>d</i>	-0.204	0.0287
$\eta$ – low organic matter, flufenacet	0.071	0.0056
$\eta$ – low organic matter, pendimethalin	0.124	0.0088
$\eta$ – medium organic matter, flufenacet	0.200	0.0125
$\eta$ – medium organic matter, pendimethalin	0.393	0.0315
$\eta$ – high organic matter, flufenacet	0.437	0.0319
$\eta$ – high organic matter, pendimethalin	0.514	0.0487

**Table 5.5.** The number of seed heads and the dry weight of that seed for plants subjected to all doses of flufenacet and pendimethalin at the pre-emergence stage on soil with varying levels of organic matter.

Soil organic matter	Number of seed heads		Dry weight of seed / g	
	Mean	SEM	Mean	SEM
Low	61.38	4.343	4.637	0.357
Medium	106.7	8.051	8.251	0.587
High	145.2	8.126	12.330	0.811

as soil organic matter and was best described by a linear model with parallel lines and different intercepts for each soil (Figure 5.3). The greater the herbicide dose at the pre-emergence stage, the lower the total plant biomass at maturity, irrespective of the active herbicidal ingredient. The soil on which it was grown, however, caused a difference in the overall size of those plants with the largest plants growing on high organic matter soil (Figure 5.3). The fact that a dose-response of total biomass was observed but with no significant effect on seed production indicates variability in partitioning of assimilate between the treatments.

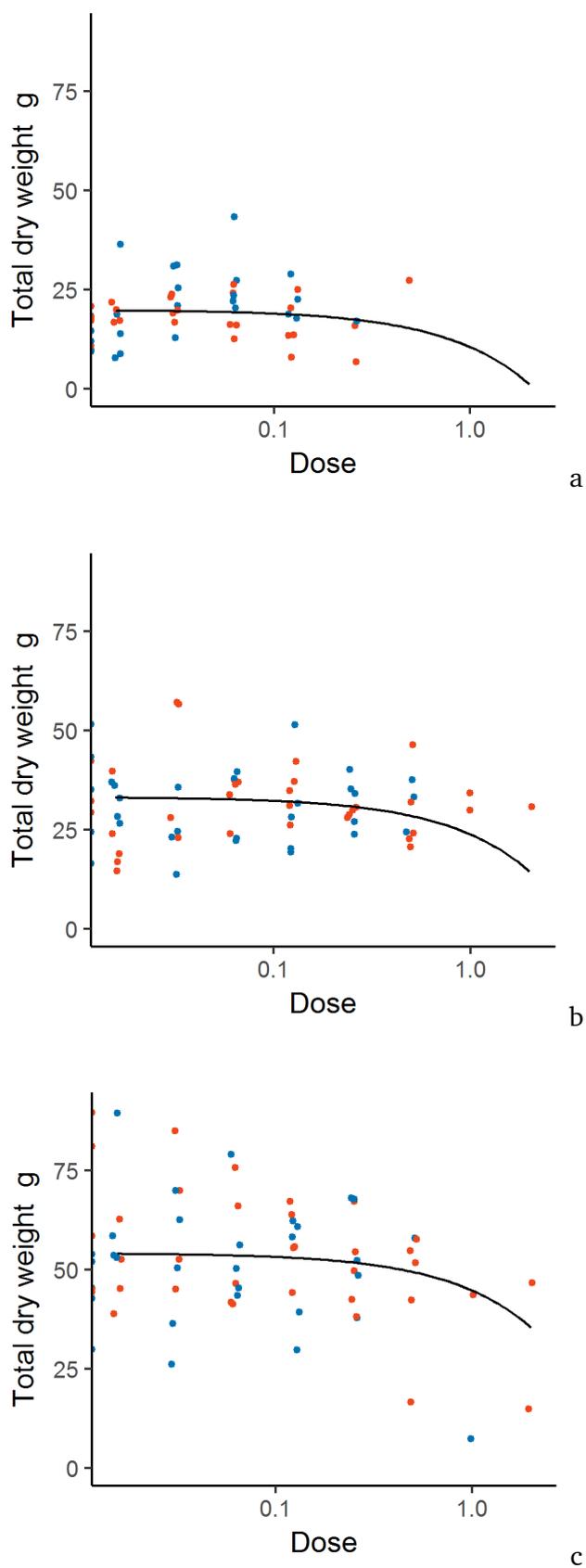


Figure 5.3. Figure legend on page 130.

**Figure 5.3.** (Figure on page 129.) The total dry weight of mature plants after the application of two pre-emergence herbicides on soil with varying levels of organic matter: (a) low, (b) medium and (c) high. Points indicate the response of each sample (flufenacet in blue, pendimethalin in red) and the fitted model is shown by a solid black line (The fit of the model was significantly improved by allowing separate lines to be fitted to each soil type yet there was no significant difference between the two active ingredients so a single line was fitted across both herbicides). Dose is given as a proportion of recommended field rate.

Seed viability was not affected by the active ingredient or dose received by the parent plant. However, a significant response to soil organic matter was detected ( $P < 0.001$ , ANOVA) with plants grown on low organic matter soil producing seed with a lower percentage of seeds germinating ( $44.7 \pm 0.14\%$ ) than those on medium ( $52.4 \pm 1.18\%$ ) or high organic matter soil ( $54.8 \pm 1.04\%$ ).

#### 5.4.1 Modelling

To predict the seed production under each treatment scenario included in our experiments (three levels of soil organic matter, two herbicides at nine doses) we used the predictions from the statistical models fitted to the survival data and the size of the seedlings at six weeks as inputs into a crop / weed competition model. As survival was not significantly affected by the choice of herbicide we adjusted survival by organic matter and dose. However, the log-logistic model describing the dose-response of seedling biomass did significantly differ according to the herbicide used and so we were able to use different inputs for flufenacet and pendimethalin here. In each case the seedling size at zero dose on each soil was used as a baseline for that soil and adjustments were made in terms of percentage size reduction. We were therefore able to simulate all three soils, both herbicides and the full range of doses, both with and without competition. The survival rates and the size reduction of individuals compared to the unsprayed plants are shown in Table 5.6.

In each case, the multiple simulations for each year generated a classic hyperbolic response curve when seed production was plotted against weed density. When crop competition was excluded there were large levels of seed production across all treatments

**Table 5.6.** The predicted proportion of seedlings surviving and the dry weight of those seedlings (as a proportion of the predicted dry weight for those that received no herbicide on the same soil type) surviving six weeks after the application of either flufenacet or pendimethalin on soil with varying levels of organic matter. Predictions for seedling survival come from a Cedergren-Ritz-Streibig model fitted to experimental data. Fitting separate lines to each soil type significantly improved the fit of the model but there was no significant difference between the two herbicides so a single line was fitted across both. Predictions for seedling dry weight come from a 4-parameter log-logistic model fitted to experimental data. Fitting separate lines to each soil type and to each herbicide significantly improved the fit of the model so separate lines were fitted to each soil x herbicide combination. Dose is given as a proportion of recommended field rate.

Herbicide Dose	Low Organic Matter		Medium Organic Matter		High Organic Matter	
	Survival	Dry weight	Survival	Dry weight	Survival	Dry weight
<i>Flufenacet:</i>						
0	0.773	1.000	0.773	1.000	0.773	1.000
1/64	0.812	0.994	0.837	1.000	0.841	1.000
1/32	0.780	0.924	0.860	0.999	0.873	1.000
1/16	0.642	0.464	0.853	0.978	0.897	0.999
1/8	0.389	0.160	0.749	0.754	0.870	0.985
1/4	0.168	0.132	0.500	0.237	0.714	0.813
1/2	0.059	0.130	0.234	0.138	0.425	0.278
1	0.019	0.130	0.085	0.131	0.180	0.141
2	0.006	0.130	0.028	0.130	0.062	0.131
<i>Pendimethalin:</i>						
0	0.773	1.000	0.773	1.000	0.773	1.000
1/64	0.812	0.999	0.837	1.000	0.841	1.000
1/32	0.780	0.991	0.860	1.000	0.873	1.000
1/16	0.642	0.876	0.853	0.998	0.897	0.999
1/8	0.389	0.354	0.749	0.977	0.870	0.992
1/4	0.168	0.147	0.500	0.742	0.714	0.890
1/2	0.059	0.131	0.234	0.231	0.425	0.381
1	0.019	0.130	0.085	0.137	0.180	0.150
2	0.006	0.130	0.028	0.131	0.062	0.132

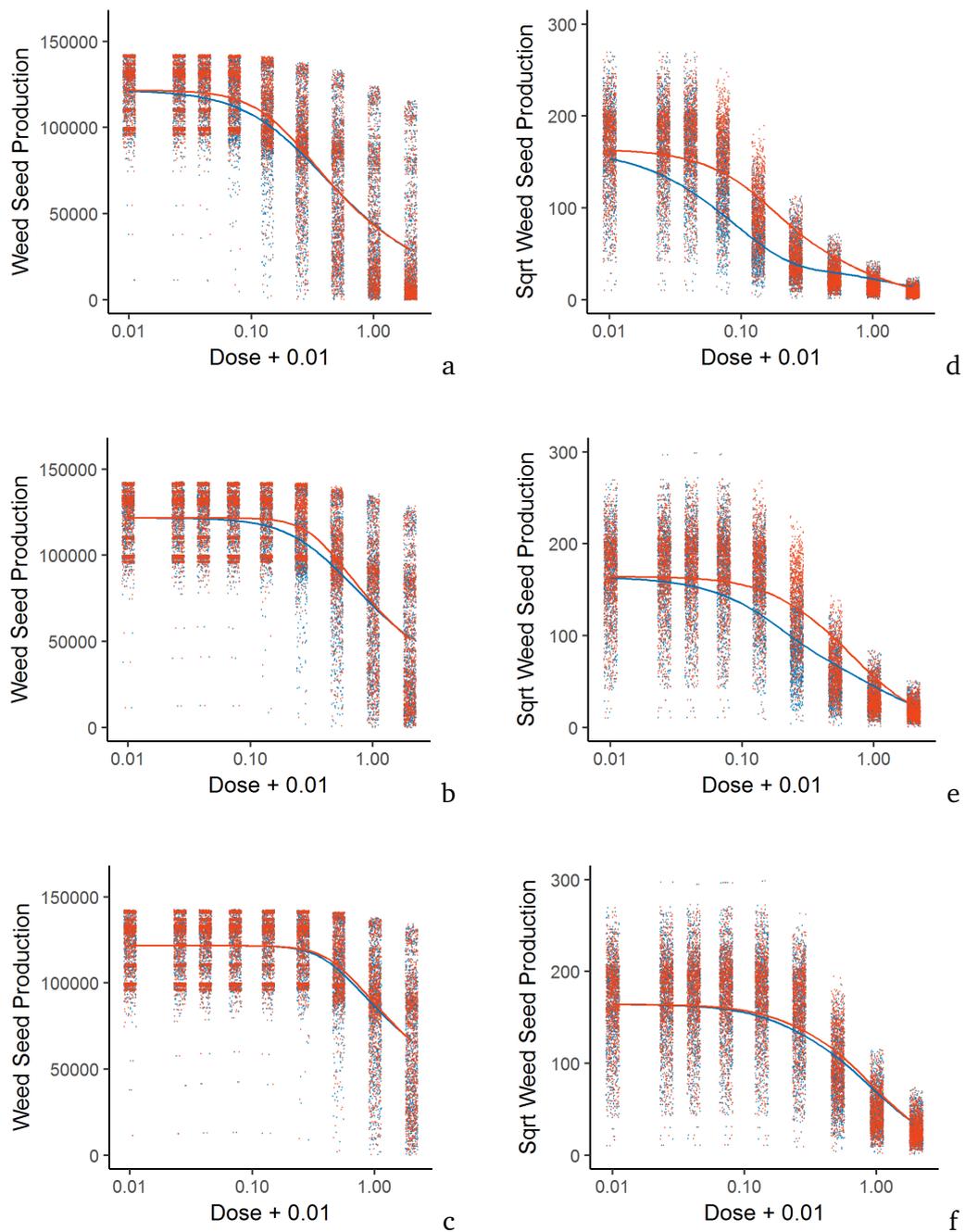
and we saw a clearly defined asymptote in seed production. Where crop competition was included in the model, weed densities were much lower and so we only observed the initial phase of this response curve and there was no asymptote in weed seed production (Supplementary Figure S5.2).

There were large inter-annual differences in the balance between crop and weed competition, which reflect the behaviour of the system in the field (Storkey & Cussans, 2007). For both the absence and presence of competition, a Cedergreen-Ritz-Streibig model (type C) best described the weed seed production. This reflects the type of model that was used for the input survival data — showing the importance of herbicide survival in the resultant seed return. The fit of the model was significantly improved in both cases (with and without crop competition) by allowing it to vary with both soil type and herbicide. This shows that sub-lethal effects of a reduced seedling size are important in determining seed return as mortality was fixed across both herbicides and so the differences seen here are only to do with sub-lethal effects.

In the model output, we observe a reduction in seed return at high doses in the absence of competition (Figure 5.4 a–c). However, the spread of the predictions from the model becomes particularly wide as the dose increases. At low doses seed production reaches an asymptote, this is particularly clear on soil with high organic matter as it is only once doses reach 1/2x field rate that we begin to see any reduction in seed return in the absence of competition (Figure 5.4 c).

When we include crop competition in the simulation model (Figure 5.4 d–f), seed production is generally much lower and we see more of a decline across a wider range of doses. It is on low organic matter soil that we observe the lowest seed production with flufenacet providing the greatest level of control. As we increase the organic matter, seed production increases and the difference between the two herbicides becomes less. When we consider the seed production at a field rate dose of herbicide we can see that whilst on low and medium organic matter soil it is fairly close to its lower asymptote, on high organic matter soil there is still a high level of seed production.

The difference in ED50s between the pot experiment and predicted seed return (Table 5.7) can be considered to be indicative of the capacity of *A. myosuroides* to compensate for the combined lethal and sub-lethal effects of the herbicides. The ED50 was generally higher for seed production than survival or seedling dry weight,



**Figure 5.4.** (Figure on page 133.) Weed seed production in the absence (a-c) and presence (d-f) of crop competition - outputs from 100 simulations for each of 10 years of weather data from the INTERCOM model across a full range of doses of herbicide application from 0 to 2x field rate on soil with varying amounts of soil organic matter: (a,d) low, (b,e) medium and (c,f) high. Points indicate the response of each model simulation and the fitted model is shown by a solid line (flufenacet in blue, pendimethalin in red). Dose is given as a proportion of recommended field rate. Seed production is on a square root scale where crop competition is included (d-f).

emphasising the importance of managing a suppressive crop canopy to support herbicide use. The lower sub-lethal effects observed on soil with high organic matter were reflected in a disproportionately greater capacity of the weeds to compensate for herbicide activity, reflecting asymmetric crop / weed competition as size differences at canopy closure are magnified through the season.

These results in combination, show us that soil with greater organic matter content generally leads to poorer control with flufenacet and pendimethalin than can be achieved on soil with less organic matter. For traits that are affected by the choice of herbicide, namely those relating to early growth, there is a greater level of efficacy achieved by flufenacet than pendimethalin, particularly on soil with lower organic matter. In the absence of competition, survivors can recover to produce large amounts of seed, in some cases (as we observed in our experiment) the same amount of seed as if no herbicide were applied. However, the simulation model showed that the reduction in size of seedlings following the application of pre-emergence herbicides leads to increased competition by the crop. Whilst this indicates that in the presence of competition the lack of sub-lethal effects observed in our experiments do not hold, it does indicate that on high organic matter soil where *A. myosuroides* seedlings can survive field-rate doses of pre-emergence herbicide it is possible for them to recover and produce non-negligible amounts of seed.

## 5.5 Discussion

Our results show that soil organic matter plays an important role in the control of *A. myosuroides* achieved by flufenacet and pendimethalin. The artificial soils used in the pot experiments reflected typical ranges of soil organic matter in UK arable fields and, although the results cannot be extrapolated directly to the field, the range of efficacies generated for the model simulations represented a realistic range for assessing the implications of variable pre-emergence herbicide activity for weed seed production.

As far as seedling survival is concerned the placement of the curve on the dose axis is altered significantly depending on the levels of organic matter in the soil. Soil with a greater concentration of organic matter shifts the dose-response curve to the right meaning a higher dose of herbicide is required to achieve the same reduction in survival.

**Table 5.7.** The predicted ED50 for seedling survival, seedling biomass and weed seed production. For seedling survival, values are obtained from the Cedergreen-Ritz-Streibig dose-response curve fitted to the experimental data (Fitting separate lines to each soil type significantly improved the fit of the model, but there was no significant difference between the two herbicides so a single line was fitted across both). For seedling biomass, values are obtained from the log-logistic dose-response curve fitted to the experimental data (separate lines were fitted for each soil type and each herbicide. For weed seed production, values are obtained for the Cedergreen-Ritz-Streibig dose-response curve fitted to the output from the crop competition model (Separate curves were fitted to each herbicide and each soil type).

Herbicide	Soil Organic Matter	Seedling Survival		Seedling Biomass		Weed Seed Production	
		ED50	SE	ED50	SE	ED50	SE
Flufenacet	Low	0.1258	0.022	0.0711	0.006	0.1226	0.002
	Medium	0.3279	0.055	0.1997	0.013	0.3330	0.004
	High	0.5466	0.088	0.4374	0.032	0.6168	0.007
Pendimethalin	Low	0.1259	0.022	0.1238	0.009	0.1577	0.002
	Medium	0.3279	0.055	0.3932	0.032	0.4465	0.005
	High	0.5466	0.088	0.5137	0.049	0.6611	0.007

Similarly, the size of the plants after six weeks is also strongly affected by soil organic matter with surviving plants grown in soil with much organic matter typically being larger than those grown in soil with less organic matter. This would indicate that on higher organic matter soil, where pre-emergence herbicides are used for *A. myosuroides* control there are likely to be more survivors than on lower organic matter soil and those surviving individuals will be larger and so more likely to be able to compete well with the crop plants. It is also likely that soil with high organic matter is better suited for *A. myosuroides* growth and competition as they have a higher capacity for moisture retention (Stratonovitch *et al.*, 2012). We would, therefore, expect an additive effect leading to enhanced weed fitness on such a soil. Further development of the model to simulate these effects of soil heterogeneity on weed growth (and also on the relationship between mature biomass and seed production) would give additional insight into the final impact of variable herbicide efficacy on weed seed production. However, we hypothesise that incorporating these processes will only further decrease the fitness penalty of sub-lethal herbicide effects for weeds growing on soils with relatively high organic matter, further emphasising the need to consider enhanced weed management on these areas of the field.

This size benefit conferred by high organic matter soil appears to hold true throughout the plants' life-cycle with plants grown in soil with higher organic matter reaching greater mature biomasses and producing more seed. In addition to this, there were few sub-lethal effects of the herbicide dose, amongst the variables we measured here in the absence of competition. Whilst soil organic matter still plays an important role we observe no cost in terms of seed production and only a small cost in terms of total biomass production to having received a higher dose of either pre-emergence herbicide. The seed produced by plants that received high doses of either pre-emergence herbicide also shows similar viability to unsprayed plants, implying that plants adjust partitioning of resources such that fecundity is not compromised. In a crop-free environment, this has no cost but would reduce competition when growing with a crop.

It is possible that sub-lethal effects of high doses of herbicides could be masked in this situation due to the use of pots rather than field studies. However, the magnitude of differences observed between the soil organic matter levels indicates that it is unlikely, at least in the low organic matter treatment, that the pots were limiting. However, further field trials could confirm this. Our modelling study shows that when competing with

a crop the reduction in biomass at the seedling stage could have severe consequences for *A. myosuroides* seed production, yet even at field-rate application of herbicide seed production is non-negligible with most seed return on high organic matter soil. Our results also indicate that this reduction in seed production across different soil types is not only due to increased competition with the crop on the different soil types but it also varies with herbicide choice as sub-lethal effects come into play.

The work we present here supports the claims of others (Blumhorst *et al.*, 1990; Nordmeyer, 2015) that pre-emergence herbicidal control is affected by soil organic matter, even within the small range of organic matters typical of the UK arable landscape. Despite this, the label recommendation for many of these herbicides suggests they remain effective up to 10% organic matter. This may have strong implications for minimal- and no-tillage systems where the aim is to increase the levels of organic matter in the topsoil as this could mean decreased levels of control by pre-emergence herbicides.

We have established here that the control of *A. myosuroides* by pre-emergence herbicides can be impacted strongly by soil organic matter, in the absence of competition. This highlights an opportunity for further research into whether these results hold true in a field situation. It also raises questions about the efficacy of other active ingredients applied to the soil as well as mixtures of multiple active ingredients across a range of soil properties. Soil moisture can also play an important role in determining the efficacy of certain herbicides. Orson *et al.* (1998) showed that *Lolium perenne* L. (perennial ryegrass) grown in pot experiments under moisture stress required a higher dose of diclofop-methyl to cause the same damage, than those with sufficient water. Blair *et al.* (1994) showed that isoproturon can give better control of *Bromus sterilis* L. (barren brome) in the fields when applied to moist soil compared with dry. The effect of weather on herbicide efficacy can also be important, however, results linking weather to efficacy can be inconsistent across years (Collings *et al.*, 2003) and so the effect of this variation on our results is something that should be considered when implementing control strategies.

In terms of impacts on *A. myosuroides* management, herbicide application by soil type is possible as many farmers have soil maps of their farms and the uptake of precision agriculture is advancing. So, in fields where there are within-field gradients of organic matter, it should be possible to adjust the application rate of the herbicide to account for this. However, it may be that further work is required to determine active ingredients

or mixtures thereof that are less impacted by soil organic matter and perhaps tailor herbicide programs to the soil properties within fields. We have also demonstrated the importance of crop competition in supporting pre-emergence herbicides in the context of a variable soil environment. This effect could be further enhanced (so reducing the capacity of weeds to compensate for sub-lethal herbicide effects) through cultural control options such as increased seed rate and the use of competitive cultivars (Andrew *et al.*, 2015). The effective combination of integrated weed management and precision weed management, therefore, cannot be achieved by studied chemical and agronomic weed control options in isolation but will require an assessment of their combined impacts across the whole growing season of the type presented in this study.

Our results supported our first hypothesis that increasing soil organic matter would lead to decreased efficacy of both flufenacet and pendimethalin in the control of *A. myosuroides*. We expect that this is due to adsorption of herbicide (Farenhorst, 2006). The differences between the two herbicides could be due to different levels of adsorption, as was described by Nordmeyer (2015) for pendimethalin and chlortoluron. Our second hypothesis was that sub-lethal doses would lead to fitness costs causing reduced growth and fecundity. We observed very little evidence of this in the experiments with only a small effect of dose on total biomass but no observable effect on seed return. However, the reduction in size at six weeks following spraying suggests that in the presence of competition we may have seen some fitness costs as the smaller seedlings may have been outcompeted in the early stages of their growth.

## 5.6 Acknowledgements

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## Chapter 6

# Modelling the Spatial Variation in Black-grass (*Alopecurus myosuroides*) due to Soil Properties

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In Chapter 3, I reported on scale-dependent relationships between *A. myosuroides* and soil properties observed in the field. These relationships were explored further with a series of pot experiments (Chapter 4 and 5) where I determined that soil organic matter, water and pH can alter the life-cycle of *A. myosuroides*, and that soil organic matter also affects the efficacy of two pre-emergence herbicides and the sub-lethal effects experienced by the plant. In Chapters 4 and 5, I demonstrated that there can be small changes to different stages of the life-cycle of *A. myosuroides* according to the soil in which it is growing. In this chapter, I initially review current approaches to modelling weed population dynamics and then describe how I developed a mechanistic model of the life-cycle of *A. myosuroides* which includes the effects of soil on the different stages of the *A. myosuroides* life-cycle that I observed in the pot experiments. The model is based on the work of Moss (1990), Paice *et al.* (1998), and Colbach *et al.* (2006a). Using

the model I tested my final hypothesis: the scale-dependent relationships between soil properties and the density of *A. myosuroides* observed in fields is an emergent property of the effect of soil on the various aspects of the weed's life-cycle. I compared simulated weed distributions to those observed in the field (Figure 3.2 in Chapter 3). I also compared the scale-dependent correlations between *A. myosuroides* and soil properties in the field (Table 3.4 in Chapter 3) with the corresponding analysis of the simulated model output. This chapter allowed me to draw together the work from all the previous chapters to address my main aim of identifying weed vulnerable zones within fields according to variation in soil properties.

The full code for the model can be found in the supplementary material.

## 6.1 Summary

The patchy nature of *A. myosuroides* distributions within fields make it an ideal candidate for site-specific weed management. However, this form of management has not been readily taken up, likely due to the risk of missing individuals that fall outside of currently mapped areas. One means by which this concern can be addressed is through the identification of “weed vulnerable zones” or areas of a field that are at risk of invasion by the weed. This can be done through the identification of associations between the weed and certain environmental properties. We have developed a spatially-explicit mechanistic model of the life-cycle of *A. myosuroides*. Soil properties vary across the field and so the response of the *A. myosuroides* life-cycle to these conditions also varies. The model was validated using data on the within-field distribution of *A. myosuroides* on commercial farms and its co-location with soil properties.

## 6.2 Modelling weed population dynamics

Field trials, monitoring and experimental data are useful for making predictions about short-term weed control or the influence of a few experimental variables. However, these are generally only applicable to a given location or time period for which they were derived and so it is often necessary to base predictions on models that capture the biological mechanisms of interest (Holst *et al.*, 2007; Freckleton & Stephens 2009).

Holst *et al.* (2007) made a comprehensive study of models of agricultural weeds. This covered 134 publications encompassing 60 weed species in 40 crops. The extent of this review demonstrates how important modelling is as a tool in weed ecology. However, they demonstrated that there are still limitations and limited use for the models that exist given that the majority of models reviewed were theoretical investigations or had only been designed to provide general guidelines. There are many advantages to taking a modelling approach when studying agricultural weeds, not only do they allow long-term predictions that would be unrealistic to obtain from field studies due to limited resources but they also allow for high levels of ecological complexity and uncertainty (Freckleton & Stephens, 2009).

There are different types of models and each will be useful for a different purpose. Empirical models are data driven and are often purely descriptive. They can support prediction but include no understanding of mechanisms and causality and so are often described as black-box models. Mechanistic models simulate processes and try to focus on causal relationships rather than correlations. Each of these types of model can be either deterministic or stochastic. A deterministic model makes definite predictions without any associated probability distributions, whereas stochastic models contain random elements or probability distributions. Stochastic models can account for uncertainties whereas the average expectation given by a deterministic model may not be the same as the average prediction from a stochastic model due to the skewed distributions for many model parameters (Freckleton & Watkinson, 1998). By modelling processes stochastically it is also possible to reduce the data requirements for model validation. Many weed models give little attention to model validation (Holst *et al.*, 2007). This is likely to be due to the large data sets required to be able to validate a model, however, it is possible to validate stochastic models with only a few data by demonstrating that they lie reasonably well within the predicted boundaries (Holst *et al.*, 2007).

We can model changes in population numbers by both deterministic and stochastic processes. Whilst all processes are ultimately deterministic, we cannot and do not need to understand them all in depth and so can model many of them stochastically. Deterministic components of weed population dynamics include predictable ecological processes whilst the stochastic components include random variations in birth and death rates as well as direct effects of environmental perturbations (Freckleton & Watkinson, 2002). It has been suggested that some weed populations may exhibit chaotic behaviour

(e.g. Wallinga & van Oijen, 1997; Gonzalez-Andujar & Hughes, 2000), if this is true then modelling them may not be able to provide useful predictions of weed abundance at the field scale; reducing or even removing their practical use (Gonzalez-Andujar & Hughes, 2000). However, Freckleton & Watkinson (2002) argued that for many weed populations this would not be the case as the system functionality required to produce this type of behaviour is not present in weed systems. They used data from the Broadbalk long-term experiment at Rothamsted Research (Thurston, 1968) to demonstrate that many weed species can persist at stable population levels and so do not demonstrate chaotic population dynamics. They also argued that if the purpose of weed models is to aid the development of control programmes then population behaviour of this kind will not affect the outcome as accurate prediction of numbers at very local scales is not necessary, rather relative changes under different management strategies are the important output.

The quantification of error in parameter estimates is often ignored in weed modelling (Freckleton *et al.*, 2008). If a weed population is close to an extinction boundary, as may be the case in a well-controlled weed population, then population densities will be highly sensitive to errors in parameter estimates making the predictions from the model considerably weaker (Freckleton *et al.*, 2008). Given a simple model of population dynamics for an arable weed, taking only seed production, germination rate, control, and density dependence into consideration, Freckleton *et al.* (2008) demonstrated that there is considerable margin for error given the error associated with any given parameter in the model. For example, if the finite rate of increase under given management conditions is determined with an error of 5% then densities can be overestimated up to threefold. Even when the estimates are unbiased and are true to the mean for the population there will be some deviation from the population mean for any given estimate.

For some given purposes of model development, errors in the estimation of model parameters may not be of particular consequence, particularly if a given management option produces drastic differences in population size, making small changes in absolute densities irrelevant to management decisions (Freckleton *et al.*, 2008). The problems associated with input error is also discussed by Gressel (2005), he outlines how incorrect assumptions in model building can lead to false conclusions being drawn and again highlights the need for model validation with field data.

There are many possible applications for weed models. One common application

is theoretical research including investigating different scenarios before the design of experiments and in order to get a deeper understanding of a system. Another common application is decision support; encompassing both general guidelines for practical weed management or specific predictions for given fields (e.g. Benjamin *et al.*, 2009 and 2010). For modelling the effect of management practices, models tend to focus on predicting the likely persistence of weeds rather than quantitative predictions of densities (Freckleton & Stephens, 2009). Often the purpose of many models is to allow the investigator to look further to the future than would be possible to predict from the outcome of field trials, this is often the case when looking at the impacts of climate change (e.g. Stratonovitch *et al.*; Garcia de Leon *et al.*, 2014) or herbicide resistance (reviewed by Renton *et al.*, 2014).

### 6.2.1 Life-cycle Models

The purpose for which a model is to be built often dictates its complexity and so many models are structured around a simple description of the weed life-cycle (Holst *et al.*, 2007). These are often based on seedbank numbers updated on a one-year time step by adding the new seeds and subtracting those that germinated or died. Moss (1990) constructed a basic model of this kind for *Alopecurus myosuroides* Huds. (black-grass) considering the life-cycle of the species and some simple descriptions of biological and ecological processes. The model is empirical and deterministic and is parameterised from various data sets from the literature. As is often the case with this type of deterministic life-cycle model based on empirical data, there are necessary assumptions about, and simplifications of the weed biology. Moss, (1990) had limited field data, particularly concerning the fate of seeds after shedding and so included germination, predation and decay within one parameter. However, this is common across many weed models, with fecundity being fixed despite its dependence on weather, weed density, crop, harvest time, and other factors (Holst *et al.*, 2007).

As with other simple weed life-cycle models, Moss (1990) ignores temporal variation (e.g due to weather), which has been shown to affect predictions of population size in a non-random way. Temporal variability in some aspects of the life-cycle, particularly fecundity, germination and survivorship leads to smaller populations than would otherwise be predicted, whilst temporal variability in weed control and competitive effects leads to larger populations than might be predicted (Freckleton & Watkinson, 1998).

To make a model fit for its intended purpose it is sometimes necessary to add complexity to this basic life-cycle model. However added complexity often comes at a trade-off with tractability of the model (Thuiller *et al.*, 2008), generally this is done by adding more detailed biology either through the inclusion of more data in empirical relationships or by detailed mechanistic modelling of biological processes and their response to the environment. Colbach and Debaeke (1998) cautioned against the black-box approach of many weed models. They argued the need for greater transparency in this type of model and suggested the life-cycle could be split into its component parts with functions considering biological and physical effects of the crop, environment and weeds.

Many models choose to concentrate on one component of the life-cycle and model it in detail, sometimes these models are generic across all weed species, specific to annuals, or will focus in on a single species. Examples of this type of model include those by Forcella *et al.* (2000) which focuses particularly on weed emergence, Benech-Arnold *et al.* (1990) on dormancy evolution, and Storkey (2004) on growth rates. However, Colbach *et al.* (2006a) were the first to incorporate all of these processes into one model: ALOMYSYS. They largely used pre-existing models and knowledge from the literature to construct their detailed model focussing on germination and emergence. Some additional experiments were done to parameterise parts of the model with further data. Their model provides a comprehensive study of the early stages of *A. myosuroides* growth and the effect of the cropping system on on the *A. myosuroides* seed bank. They validated the model in a field trial where *A. myosuroides* seeds were introduced to a field that was known to be free of *A. myosuroides* (Colbach *et al.*, 2006b). Emergence and seed survival were measured and compared to model predictions. Emergence predictions were generally accurate both in terms of timing and magnitude of the flushes. However, seedling mortality was often underestimated, particularly in compacted plots, and seed survival at shallow depths was generally over predicted. The ALOMYSYS model was later updated to include further submodels detailing the life-cycle from seedling to seed production using data from glasshouse experiments and field trials (Colbach *et al.*, 2007). The model was shown to accurately simulate seedling densities from a field trial and accurately ranked different cropping systems in terms of their capacity for weed control.

## 6.2.2 Spatial Structure in population dynamics

Most weed population dynamics models ignore the within-field distribution of the weed and generally simulate the average density per area (Holst *et al.*, 2007). However, some studies include the spatial distribution of weeds. Developing spatially explicit models is difficult due to the necessity of obtaining dispersal data and data on the impact of environmental heterogeneity on individual performance (Freckleton *et al.*, 2008) yet, as many weed species are patchy, it is often desirable to include their spatial distribution in models of their population dynamics. These models often only include intrinsic demographic parameters and dispersal. These features alone are often not sufficient to describe the degree of patchiness observed. It is thought that this may be due to the omission of soil variables (Paice *et al.*, 1998; Rew & Cousens, 2001). Also, dispersal models are often weak predictors as it is difficult to determine the exact shape of the dispersal kernel; an important part of modelling patch spread (Rew & Cousens, 2001).

The incorporation of spatial structure into weed population dynamics models can also have an important stabilizing effect, yet it is often ignored (Freckleton *et al.*, 2008). The densities within individual patches can be relatively high despite low densities across the whole field. This makes the error in estimation of model parameters becomes less problematic as the problems associated with small errors in parameter estimates when a population is close to an extinction boundary will be buffered by the high population densities in the centre of patches and so stability is maintained (Freckleton *et al.*, 2008).

Paice *et al.* (1998), considered the need for a spatial component to models of *A. myosuroides* population dynamics. Building on basic models of the *A. myosuroides* life-cycle they incorporated elements of stochasticity into the life-cycle processes as well as binomial probability of herbicide survival. They included both isotropic and anisotropic dispersal processes derived from Howard *et al.* (1991) and modelled this in a rectangular area of a field defined by square cells scalable to real units of distance. They showed that when dispersal only occurs over short distances, patchiness can be maintained and even if the field is initialised with a uniform seed bank the population will develop toward a more patchy distribution.

Gonzalez-Andujar *et al.* (1999) also considered spatial patterns in the modelling of *A. myosuroides* in an array of hexagons representing part of a field. The centre of each cell was spaced 1 m from its neighbours. Dispersal was assumed to be isotropic

and followed an exponential distribution truncated at 2.5 m. Isotropic dispersal by the combine was also considered. They demonstrated through simulations that there was some evidence for patch longevity (<10 years) under these conditions but that without further intervention a uniform distribution would be reached eventually.

### 6.2.3 Environment

The abiotic environment is often ignored in weed population models, despite the importance of factors such as light, water and nutrients, and intra- and interspecific competition (Holst *et al.*, 2007). Often, the importance of the environment is outweighed by its complexity. Models usually operate on a yearly time-step. This precludes much environmental variation, which generally operates at shorter time steps.

Dunker *et al.* (2002) took steps toward including soil in a spatial model of *A. myosuroides* population dynamics. They included nutrients, soil pH and particle size in their model, based on the results of a pot experiment where these were manipulated in artificial soils. They verified this model in one field where *A. myosuroides* counts and soil properties were measured on a 50 x 50 m grid. Their model was based on the demographic data from Moss (1990). Only germination probability and probability of survival were affected by soil in their model as their experiment on which these were based was only conducted for 5 weeks post germination. The model arena consisted of a 20 x 20 m grid and the population dynamics continued independently in each cell. One percent of seeds from each cell were dispersed equally into the 4 adjoining cells. They found their simulations to be only weakly correlated with the real data and only 4 out of 20 showed a significant correlation, yet 18 out of the 20 simulations produced stronger correlations when soil properties were included.

## 6.3 Introduction

*Alopecurus myosuroides* Huds. (black-grass), is a common grass weed of winter cereals in north-west Europe (Holm *et al.*, 1997). It is particularly problematic in the UK due to its fast reproductive rate and strong competitive ability with the crop (Maréchal *et al.*, 2012). Its life-cycle is largely synchronised with that of winter cereals allowing it to compete at all stages of growth (Maréchal *et al.*, 2012). *Alopecurus myosuroides* plants

can produce vast amounts of seeds (Moss, 1980) meaning small failures in control can lead to rapid population growth and dense infestations within some fields. As such, control of the population is of great importance to farmers. Currently, the main means by which farmers choose to control this pernicious weed is through broadcast application of herbicides. However, many farmers have seen a decline in the levels of control achieved because of the evolution of herbicide resistance. This together with the decreasing number of chemical products available for use and increasing economic and environmental pressures to reduce herbicide use puts a growing emphasis on the optimisation of current techniques and finding alternative approaches (Grundy, 2003).

Approaches for reducing the amount of herbicide on farm are wide ranging, from the introduction of additional cultural control methods focussing on the species' biology and ecology, to the introduction of economic thresholds or particular densities of weeds below which there is little economic reason to spray herbicides as the cost of inputs will exceed yield losses. Another option, which is gathering interest, is precision management, including the spatially variable application of herbicides, or patch spraying.

The within-field distribution of *A. myosuroides* is patchy (Wilson & Brain, 1991; Krohmann *et al.*, 2006; Metcalfe *et al.*, 2016 and 2017c (Chapters 2 and 3)) and as such this presents an opportunity for site-specific management. There are currently two main approaches to patch management: real-time detection of weeds and treatment maps. Each of these approaches has merit but also associated problems. The use of real-time sensors is an approach that is still in development, and whilst already feasible it is not yet at the stage of widespread commercialization (e.g. Murdoch *et al.*, 2010 and 2014), whereas treatment maps can be created more easily from manually sampled data on weed distributions, but can sometimes be of inadequate quality, often because the sampling on which they are based was too sparse (Metcalfe *et al.*, 2016 (Chapter 2)). Both approaches are based on the mapping of easily detectable seed heads in the summer. However, Metcalfe *et al.* (2017c (Chapter 3)) showed that the distribution of seed heads in the summer is a contraction of the initial *A. myosuroides* patch and so spray maps based upon these distributions present a risk of missing the true extent of the seedling patch. This risk of missing individuals that fall outside of mapped zones is perhaps the biggest hurdle in the implementation of patch spraying on farms due to the inherent and understandable conservativeness of farmers when it comes to weed control. Given the consequences of a control failure, the concept of leaving some areas of the field

unsprayed is currently seen as an unacceptable risk.

A possible extension to current techniques which addresses concerns about individuals establishing outside of mapped patches is to identify parts of the field that are vulnerable to *A. myosuroides*. These “weed vulnerable zones”, once identified could be used in the creation of spray maps to guide the precision application of herbicides. As there is some indication that the patchy distribution of *A. myosuroides* in fields is related to variation in soil properties (Holm *et al.*, 1997; Lutman *et al.*, 2002, Murdoch *et al.*, 2014, Metcalfe *et al.*, 2016 and 2017c (Chapters 2 and 3)). This may provide a basis upon which to identify weed vulnerable zones within fields. If it is possible to identify a deterministic link between the soil and the location of *A. myosuroides* patches then soil maps could be used as a basis for patch spraying. Many farmers will already have soil maps for their farms and may already be using these in other forms of precision management such as the variable application of fertiliser within-field.

### 6.3.1 Objectives

Our aim was to develop a spatially explicit model of the life-cycle model of *A. myosuroides*. The model was based on the work of Moss (1990), Colbach *et al.* (2006a) and Paice *et al.* (1998) but extended to include the direct and indirect effect of soil on the weed based on experimental data. By modifying the life-cycle of the plant according to known responses to variation in soil properties we tested the hypothesis that scale-dependent relationships between soil properties and the density of *A. myosuroides* observed in fields by Metcalfe *et al.* (2017c (Chapter 3)) can be modelled according to the changes to each aspect of the weed’s life-cycle caused by different soil properties.

## 6.4 Model Implementation

**Table 6.1.** Nomenclature used in Chapter 6.

Parameter	Description
<b>Soil properties</b>	
$D_b$	Bulk density
$S_{\text{Clay}}$	Soil clay content
$S_{\text{GWC}}$	Soil gravimetric water content
$S_{\text{Silt}}$	Soil silt content
$S_{\text{SOM}}$	Soil organic matter
$S_{\text{VWC}}$	Soil volumetric water content
<b><i>A. myosuroides</i> Emergence</b>	
$a$	Lag phase of germination
$A$	Age of the seed
$c$	Germination shape parameter
$D$	Depth of seed
$G$	Proportion of seeds that germinate
$M$	Maximum level of germination
$M_S$	Mean seed mass
$N$	Total available nitrogen
$T$	Daily temperature
$t_a$	Germination lag phase offset
$T_b$	Base temperature
$t_{\text{DH}}$	Hydrothermal time spent in darkness prior to tillage
$t_{\text{GM}}$	Time from germination to maturity of the mother plants
$W_{\text{def}}$	Water deficit between flowering and maturity
$x_{50}$	Time to 50% germination
$\theta_{\text{H}}$	Hydro time
$\theta_{\text{HT}}$	Hydrothermal time
$\theta_{\text{T}}$	Thermal time
$\psi$	Daily water potential
$\psi_b$	Base water potential
<b>Herbicide Mortality</b>	
$p$	Probability of surviving pre-emergence herbicide application
$P(i)$	Probability of $i$ plants surviving pre-emergence herbicide application
$t$	Initial number of plants in a cell
$\zeta$	Parameter in relationship between soil organic matter and survival
$\eta$	Parameter in relationship between soil organic matter and survival
$\tau$	Parameter in relationship between soil organic matter and survival

**Table 6.1** continued overleaf

Table 6.1 continued

Parameter	Description
<b>Seed Production</b>	
$D_{\text{Heads}}$	Density of heads
$D_{\text{Plants}}$	Density of plants
$F_{\text{TSW}}$	Fraction of transpirable soil water
$H_1$	Number of heads when there is one plant
$T_{A:P}$	Ratio of actual to potential soil transpiration
$\alpha$	Parameter in relationship between plant and head densities
$\beta$	Parameter in relationship between plant and head densities
$\xi$	Parameter in relationship between soil organic matter and the number of heads per plant
$\epsilon$	Parameter in relationship between the fraction of transpirable soil water and the ratio of actual to potential soil transpiration
$\omega$	Parameter in relationship between soil organic matter and the number of heads per plant
$\varsigma$	Parameter in relationship between soil organic matter and the number of heads per plant
$\rho$	Parameter in relationship between the fraction of transpirable soil water and the ratio of actual to potential soil transpiration
<b>Seed Dispersal</b>	
$c_t$	Transition point between Gaussian and exponential components of dispersal by the combine and cultivation
$f(x, y)$	Dispersal probability function
$P(m, n)$	Probability of a seed falling into a cell at the distance from the source $x = m, y = n$
$S$	side length of the cell (m)
$x$	Distance from the starting plant
$\gamma$	Parameter in distribution for dispersal by combine and cultivation
$\epsilon$	Parameter in distribution for dispersal by combine and cultivation
$\lambda$	Parameter in distribution for dispersal by combine and cultivation
$\mu$	Mean of distribution used for natural dispersal
$\sigma$	Standard deviation of distribution used for natural dispersal

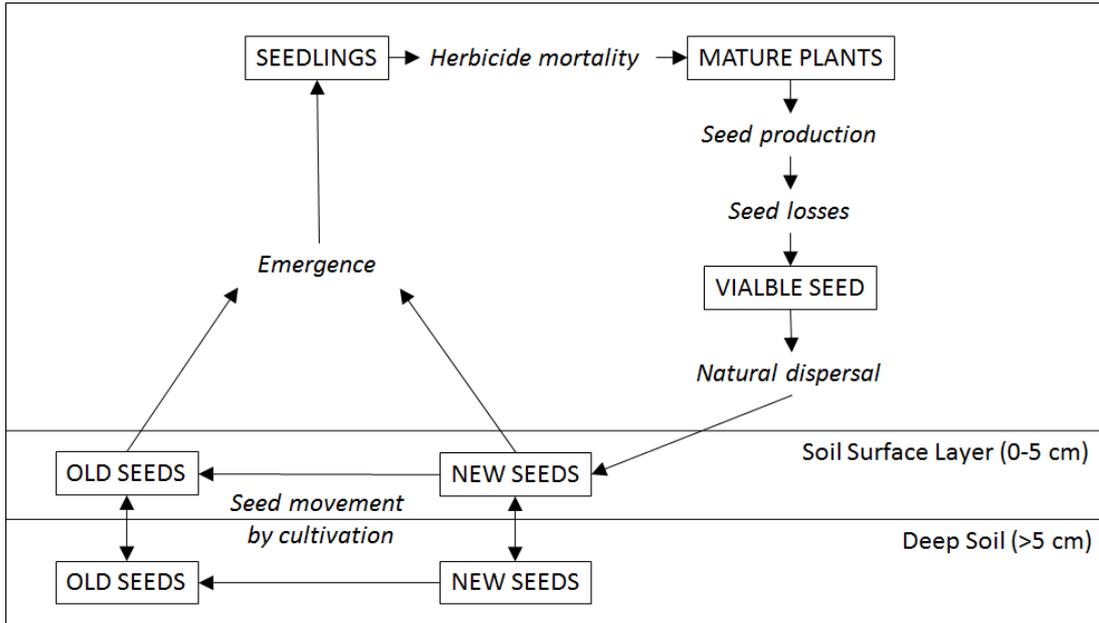
Table 6.1 continued overleaf

Table 6.1 continued

Parameter	Description
<b>Scale-dependent correlations</b>	
$g$	standard normal distribution
$L$	Lower triangular matrix obtained from the decomposition of the covariance matrix for the simulated field
$m$	Mean of all simulated soil values for a given soil property
$m_{\text{obs}}$	Mean of the observed data for a given soil property
$R$	Conditioning data for soil simulation
$s$	Standard deviation of all simulated soil values for a given soil property
$S$	Unsampled positions for soil simulation
$s_{\text{obs}}$	Standard deviation of the observed data for a given soil property
$x$	A simulated soil value
$y$	Vector of conditionally simulated values
$z$	Standard normal form of the conditioning data for soil simulation

We developed a spatially explicit model of *A. myosuroides* population densities within a field incorporating various processes throughout the plant's life-cycle (Figure 6.1). There are four main stages to the life-cycle: seedlings, mature plants, viable seed and the seed bank, these are connected by various processes relating each stage to the next (see Figure 6.1). The modelled field is described by a grid of square cells, the side length of which can be defined in real units of distance. We define the relative position of these cells in Cartesian coordinates and so a rectangular area of defined size can be simulated allowing spatial processes, such as dispersal, between cells. The life-cycle component of the model follows Moss (1990), and uses the parameterisation for various aspects of the life-cycle from that original work, with stochastic components added. The life-cycle runs independently in each grid cell with various processes being affected by the soil properties associated with that cell adjusted according to the results of the experiments in Chapters 4 and 5. In each iteration of the model (on a yearly time step) there are two cohorts of seeds in each of two soil layers; new seeds (shed in the previous year) and old seeds (shed in any year prior).

We initiate the model with weather data from Rothamsted met station (Hertfordshire, UK) beginning with data from 1966 and load subsequent yearly weather data in chronological order. Each weather set contains daily measurements for solar irradiation ( $\text{kJ m}^{-2} \text{d}^{-1}$ ), minimum and maximum temperatures ( $^{\circ}\text{C}$ ), wind speed ( $\text{m s}^{-1}$ ),



**Figure 6.1.** Basic component structure of the spatially explicit life-cycle model of within-field *A. myosuroides* population dynamics. Processes are shown in italics and components of the *A. myosuroides* life-cycle are boxed and capitalised.

precipitation ( $\text{mm d}^{-1}$ ) and sunlight (hours).

#### 6.4.1 Soil Properties

For each grid cell we set values for clay content (%), silt content (%), pH, organic matter (%), gravimetric water content (%), slope, and aspect, at a resolution consistent with the chosen grid size. We then calculate sand content (clay, silt and sand sum to 100%) and bulk density. The bulk density ( $\text{g cm}^{-3}$ ,  $D_b$ ) was calculated using the pedotransfer function:

$$D_b = 0.80806 + 0.823844 \exp(-0.27993 S_{\text{SOM}}) + 0.0014065 (1 - S_{\text{Clay}} - S_{\text{Silt}}) - 0.0010299 S_{\text{Clay}} \quad (6.1)$$

derived by Hollis *et al.*, (2012) for cultivated topsoil, where  $S_{\text{SOM}}$  is the soil organic matter (%),  $S_{\text{Clay}}$  is the soil clay content (%) and  $S_{\text{Silt}}$  is the soil silt content (%).

Initial values of soil gravimetric water content ( $S_{\text{GWC}}$ ) were then converted to

volumetric water content ( $S_{VWC}$ ) by

$$S_{VWC} = \frac{S_{GWC} \times D_b}{100}. \quad (6.2)$$

We modelled the change in volumetric water content of the soil on a daily time step with additions from daily precipitation and losses from evapotranspiration. Evapotranspiration was calculated for a bare soil surface in the autumn, and a crop canopy at other times of the year. For these calculations we followed the analysis by Penman (Frere & Popov, 1979; Penman, 1948, 1956, and 1963). The Penman formulae are dependent on the evaporative demand of the atmosphere and the net absorbed radiation, which are calculated using temperature, irradiation and wind speed from the daily weather data sets. Other required values including reference values for albedo and constants used in the formulae were taken from FAO guidelines for computing crop water requirements (Allen *et al.*, 1998).

In order to use the inputted topography data to compute solar irradiation (shown to be an important determinant of *A. myosuroides* patch location in Chapter 3) we first split the daily irradiation into its direct and diffuse component parts according to the latitude (Kropff, 1993; Kropff *et al.*, 1993). Each cell, irrespective of topography, received the full amount of diffuse irradiation, but the direct component was modified according to the slope and aspect of the field in each cell by scaling it up or down relative to a reference value for a flat field so that steep south facing slopes received more direct radiation than shallow or north facing slopes (Frank & Lee, 1966).

Water potential of the soil varies with soil type. We calculate this using the van Genuchten pedotransfer function (van Genuchten, 1980), which uses known soil properties to calculate the water potential. If the water potential exceeds 15000 mbar then we assume the field has reached wilting point and no more water can be lost. Conversely if the water potential drops below 50 mbar then the field is at capacity and any additional water input will drain through and so the water content of the soil does not increase.

## 6.4.2 Management

We implemented the option to add a break crop in any chosen years. This prevents any plants from growing in that year and so prevents seed return, seeds are still moved

within the soil due to cultivation. The type of cultivation used each year can also be changed between ploughing and tining to <5, 10 or 20 cm. This affects the proportions of seeds moved between soil layers at cultivation, as explained below.

The Julian day of cultivation, *A. myosuroides* flowering and harvest are chosen each year by sampling from a normal distributions with means 258, 150, and 206 and variances 8, 3, and 6 respectively (data from Storkey & Cussans, 2007).

### 6.4.3 *A. myosuroides* Emergence

Colbach *et al.* (2006a) model the proportion of seeds that germinate ( $G$ ) using information about the seeds, such as the age of the seed (days,  $A$ ), time from germination to maturity of the mother plants (days,  $t_{GM}$ ), water deficit between flowering and maturity (mm,  $W_{def}$ ), depth of seed (cm,  $D$ ), hydrothermal time spent in darkness prior to tillage ( $t_{DH}$ ), mean seed mass (g,  $M_S$ ), and total available nitrogen (kg ha<sup>-1</sup>,  $N$ ). They describe  $G$  as a function of hydrothermal time ( $\theta_{HT}$ ):

$$G = M \left[ 1 - e^{\left( \frac{-k(\theta_{HT}-a)}{x_{50}-a} \right)^c} \right] \quad \text{when } \theta_{HT} > a$$

$$G = 0 \quad \text{otherwise} \quad (6.3)$$

where  $M$ , the maximum level of germination, is given by

$$M = M_0 \frac{0.5311 - 0.00947 D}{0.5311} \exp(-0.00115 t_{DH}^{1.121}) \quad (6.4)$$

where

$$M_0 = 0.924 - 0.000149 t_{GM} + 0.391 e^{-0.033 A} - 0.00380 t_{GM} e^{-0.033 A} + 0.00077 W_{def}. \quad (6.5)$$

The parameter  $a$ , which is the lag phase of germination, is given by

$$a = 0.95664 \frac{1}{v_m} a_0 \quad (6.6)$$

where

$$a_0 = 49.78 - 66.43 e^{-0.0086 A} - 0.0022 t_{GM} + 0.358 t_{GM} \cdot e^{-0.0086 A} \quad (6.7)$$

and

$$v_m = \frac{0.5311 - 0.00947 D}{0.5311}. \quad (6.8)$$

The shape parameter  $c$  is given by

$$c = 0.95664 v_m c_0 \quad (6.9)$$

where

$$c_0 = 0.125 - 1.997 e^{-0.063A} + 0.00676 t_{GM} + 0.0199 t_{GM} e^{-0.063A} + 0.0101 W_{def} + 246.9 M_S - 0.00702 N \quad (6.10)$$

and the time to 50% germination,  $x_{50}$ , is given by

$$x_{50} = \frac{1.04533}{v_m} x_0 \left( e^{0.212 t_{DH}^{1.121}} - 1 \right) \quad (6.11)$$

where

$$x_0 = 65.72 + 200.99 e^{-0.044A} + 0.0968 t_{GM} - 1.086 W_{def} \quad (6.12)$$

We used information about the seeds from Experiment 1 in Chapter 4 (Table 6.2) to see if this model fitted our data.

Using Colbach *et al.*'s parameterisation (2006a) as described above, Equation 6.3 accurately recreated the shape of the curve for our data (Figure 6.2) but the lag phase was not large enough. In order for the lag phase to match our data we added an offset ( $t_a = 49.169$ ) into Equation 6.3 giving

**Table 6.2.** Starting conditions used to check suitability of equations in Section 6.4.3 for modelling germination rates. These conditions are estimated for the seeds used in Experiment 1 in Chapter 4.

Seed characteristic/environmental condition	Parameter	Estimate for seed used in experiment
Age of the seed (days)	$A$	817.5
Time from germination to maturity of the mother plants (days)	$t_{GM}$	297.5
Water deficit between flowering and maturity (mm)	$W_{def}$	0.0
Depth of seed (cm)	$D$	1.5
Hydrothermal time spent in darkness prior to tillage	$t_{DH}$	425.0
Mean seed mass (g)	$M_S$	0.0014
Total available nitrogen (kg/ha)	$N$	25.0

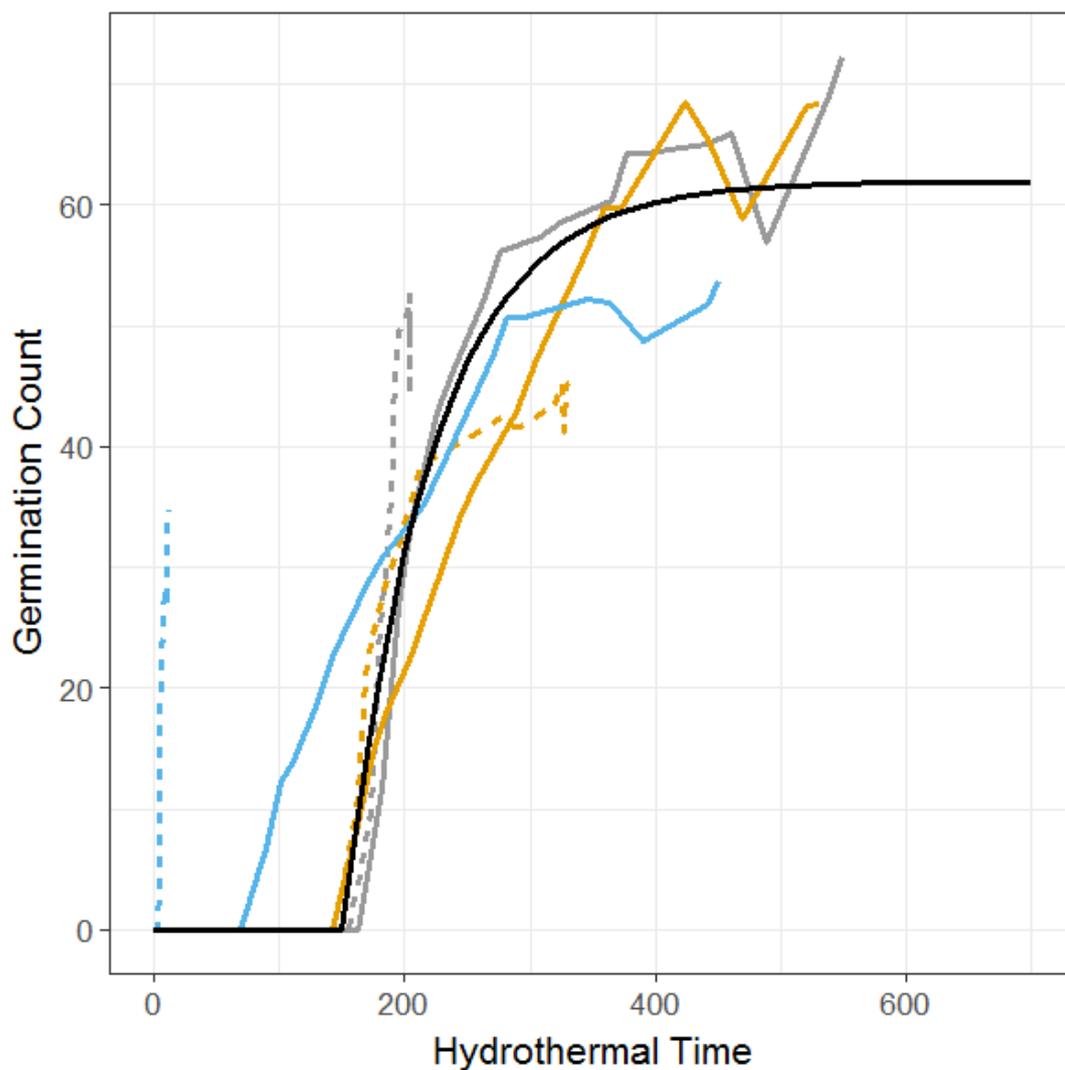
$$G = M \left[ 1 - e^{\left( \frac{-k(x-t_a-a)}{x_{50}-a} \right)^c} \right] \quad \text{when } x > a + t_a$$

$$G = 0 \quad \text{otherwise} \quad (6.13)$$

The offset increased the delay before the commencement of germination to match the mean delay for the four treatments that acted in a similar manner (Figure 6.2). This did not include the highest organic matter soil (shown in blue), as we believe that due to the artificial nature of this soil we were not able to accurately measure the soil moisture content and so the plotted accumulation of hydrothermal time is likely to be incorrect (Figure 6.2).

As our experimental data supported the use of this model (Equation 6.13 parameterised by Equations 6.4–6.12) we used it to model seedling emergence. We assumed the age ( $A$ ) of the old cohort of seeds was 818 days and the new cohort was 60 days. Changing this parameter allowed the germination of seeds to occur at different rates. We calculate the water deficit ( $W_{def}$ ) experienced by the parent plants from the previous flowering to previous harvest by taking the difference between the daily evapotranspiration and the sum of the soil water content and daily precipitation. If more water is lost to evapotranspiration than is available then this difference is added on to the water deficit.

Hydrothermal time ( $\theta_{HT}$ ) is accumulated from the day of cultivation on a daily time step by



**Figure 6.2.** Germination data plotted against hydrothermal time for data obtained from Experiment 1 in Chapter 4. Grey is low organic matter, Yellow is medium organic matter and blue is high organic matter. Solid lines show high water input data and dashed lines are low water input. The solid black line shows the resulting germination counts from Equation 6.13 when parameterised as described in Table 6.2.

$$\theta_{HT} = \theta_H \theta_T \quad (6.14)$$

where

$$\begin{aligned} \theta_H &= \psi - \psi_b \quad \text{if } \psi > \psi_b \\ \theta_H &= 0 \quad \text{otherwise} \end{aligned} \quad (6.15)$$

and

$$\begin{aligned} \theta_T &= T - T_b \quad \text{if } T > T_b \\ \theta_T &= 0 \quad \text{otherwise} \end{aligned} \quad (6.16)$$

$\psi$  is the daily water potential and  $T$  is the daily temperature.  $\psi_b$  and  $T_b$  are the base water potential and temperatures required for germination respectively. Following Colbach *et al.* (2002a and b) we set these to  $\psi_b = -1.53$  and  $T_b = 0$ . The accumulation of hydrothermal time from cultivation continues until either the green area index of the wheat (GAI) reaches 0.5 or for a maximum of 50 days. GAI is calculated using a function from Storkey & Cussans (2000) which uses empirically derived information about the growth rate of wheat plants.

Germination data on different levels of soil pH (Metcalf *et al.*, 2017b (Experiment 2 in Chapter 4)) indicate that the asymptote for germination is higher when soil pH is low. As we only had data for two different pH we included a pH threshold of 6.5 below which  $M$  (Equation 6.3) is multiplied by the ratio of the values for the asymptote for the fitted curve for the low and high pH treatment respectively (40.92/36.72) (Metcalf *et al.*, 2017b (Table 4.4 in Chapter 4)).

We calculate the number of seedlings by taking the number of new seeds in the soil surface layer and multiply this by the proportion of new seeds germinating and adding this to the number of old seeds in the same layer multiplied by the proportion of old seeds germinating).

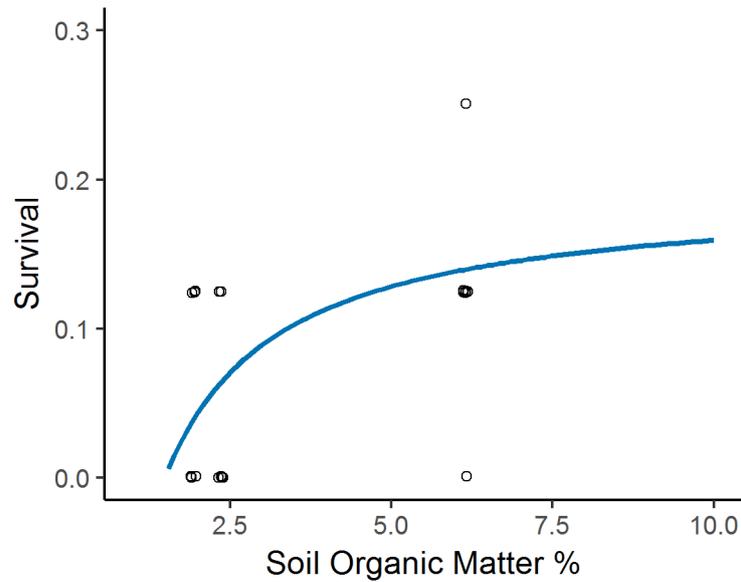
#### 6.4.4 Herbicide Mortality

We modelled the survival rate of *A. myosuroides* after the application of pre-emergence herbicides using data from Metcalf *et al.* (2017a (Chapter 5)). We took the data points for the proportion of seedlings surviving either herbicide tested (flufenacet or

pendimethalin) when a dose equivalent to field rate was applied. We then plotted this against the organic matter (%) in the soil and fitted the equation

$$\text{survival} = \frac{\eta S_{\text{SOM}}}{1 + \zeta S_{\text{SOM}}} + \tau, \quad (6.17)$$

where  $S_{\text{SOM}}$  is the percentage soil organic matter and  $\eta$ ,  $\zeta$  and  $\tau$  are parameters to be fitted. The fitted values were  $\eta = 4.9$ ,  $\zeta = 3.8252$ , and  $\tau = -1.0890$  (Figure 6.3).



**Figure 6.3.** Relationship between soil organic matter and survival after the application of pre-emergence herbicide. The discs are data from Chapter 5 and the blue fitted curve is the optimised form of Equation 6.17.

In the model, the probability of survival ( $p$ ) is then taken from this fitted curve for a given soil organic matter and the number of plants surviving is drawn from a binomial distribution:

$$P(i|t, p) = \binom{t}{i} p^i (1-p)^{t-i} \quad (6.18)$$

where  $P(i)$  is the probability of  $i$  plants surviving from an initial number of  $t$  plants in the cell.

Similarly, we also draw the number of plants surviving application of post-emergence herbicides from a binomial distribution of the same form with a 0.3 probability of survival (Bayer CropScience, 2017) — this is independent of soil properties.

### 6.4.5 Seed Production

Seed-head production has been shown to be dependent on plant density (Moss *et al.*, 2010). At high plant densities, the number of heads ( $\text{m}^{-2}$ ,  $D_{\text{Heads}}$ ) reaches an asymptote despite increasing plant numbers ( $D_{\text{Plants}}$ ):

$$D_{\text{Heads}} = \frac{\beta D_{\text{Plants}}}{1 + \alpha D_{\text{Plants}}} \quad (6.19)$$

Moss *et al.*, (2010) parameterised this equation with data from 462 plots in 16 field experiments to give values of  $\beta = 8.71$  and  $\alpha = 0.005741$ . In our experiment looking at the effect of soil organic matter on head production (Experiment 1 in Chapter 4) we only had one plant and so we would not expect this to be representative of the number of heads produced under field conditions. However, we can still consider the relative differences in head production on contrasting soil types. We compared the average number of heads per plant for each treatment to the average value across the whole experiment to give a scaling factor. We then scaled the value produced by Equation 6.19 for one plant by this value to give the expected number of heads for each treatment under field conditions. We then parameterised the equation for each of our experimental soil types. We had no reason to assume that the asymptote might change with soil and so we kept this constant at

$$\text{asymptote} = \frac{\beta}{\alpha} = 1517.157 \quad (6.20)$$

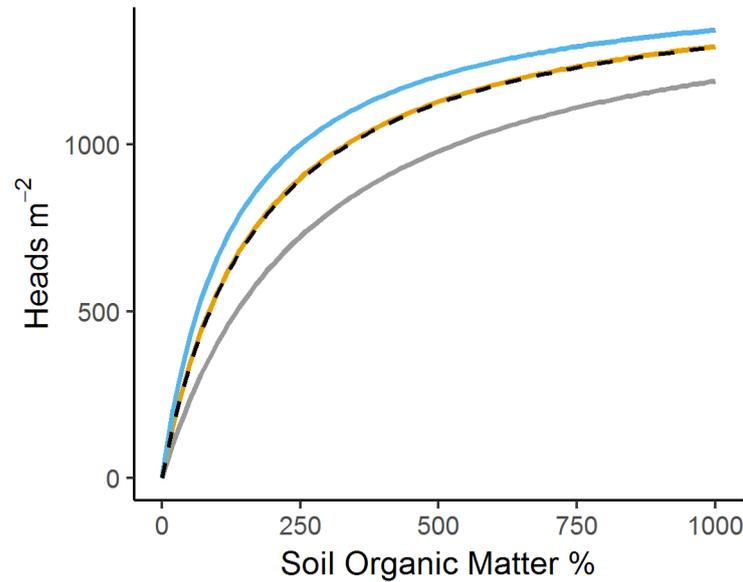
We then rearranged to find  $\alpha$  and  $\beta$  by substituting in the number of heads when there is one plant ( $H_1$ )

$$\alpha = \frac{H_1}{1517.157 - H_1} \quad (6.21)$$

$$\beta = 1517.157 \alpha \quad (6.22)$$

When we parameterised the curve in this manner for the scaled mean value at one plant for each of the three soil properties in our experiment (Chapter 4) we got different curves for each organic matter all reaching the same asymptote but with different slopes (Figure 6.4). On the highest organic matter the number of heads increased rapidly with

the number of plants, whereas on low organic matter the number of heads increased more steadily as plant numbers increase. On the medium organic matter, we saw a response very like that observed by Moss *et al.* (2010), for which they provided the original parameterisation of the equation.



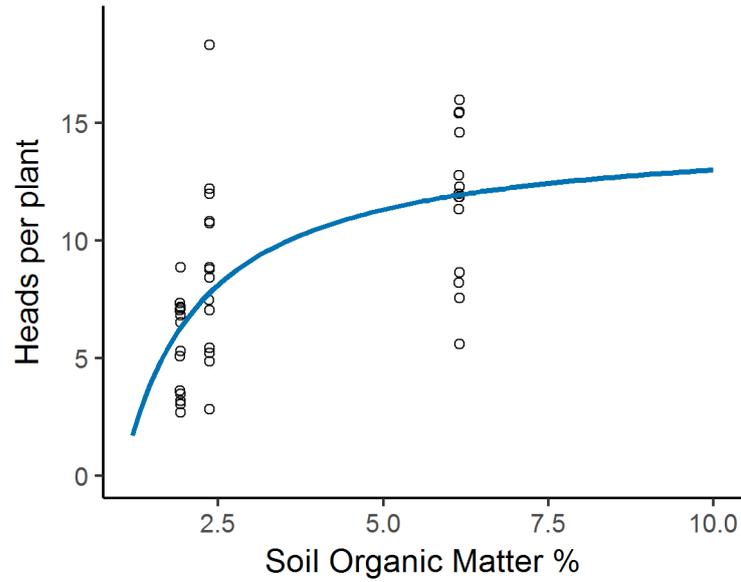
**Figure 6.4.** Density dependent relationship between plants and heads ( $\text{m}^{-2}$ ) with curve parameters  $\beta$  and  $\alpha$  adjusted according to soil organic matter. The relationship and parameterisation described by Moss *et al.* (2010) is shown by a dashed black line, grey is low organic matter; yellow is medium organic matter and blue is high organic matter.

To make this relationship more general across a range of soil organic matter contents we plotted all the original data values for the number of heads per plant at the three levels of organic matter (Figure 6.5) and fitted a curve

$$H_1 = \frac{\xi S_{\text{SOM}}}{1 + \omega S_{\text{SOM}}} + \varsigma \quad (6.23)$$

where  $S_{\text{SOM}}$  is the percentage soil organic matter, and  $\xi$ ,  $\omega$ , and  $\varsigma$  are the parameters fitted to the data. The fitted values were  $\xi = 844.4883$ ,  $\omega = 6.9542$ , and  $\varsigma = -106.7242$  (Figure 6.5).

We used this relationship to find  $\alpha$  and  $\beta$  (Equations 6.21 and 6.22) and then used Equation 6.19 to give a density dependent relationship between plants and heads ( $\text{m}^{-2}$ ) on any given amount of soil organic matter.



**Figure 6.5.** Relationship between soil organic matter and the number of heads per plant. The black discs are data from Chapter 5 and the blue line is the curve fitted is from Equation 6.23.

Water stress is known to affect plant yield (Osakabe *et al.*, 2014) and so we reduced the number of heads produced by the process described above according to the ratio of actual to potential soil transpiration ( $T_{A:P}$ ) over the growing season. This is given by

$$T_{A:P} = \frac{1}{1 + \epsilon \exp(\rho \times F_{TSW})} \quad (6.24)$$

where  $\epsilon$  and  $\rho$  are parameters derived for *A. myosuroides* from a series of glasshouse experiments (Storkey & Cussans, 2007). We calculated the fraction of transpirable soil water ( $F_{TSW}$ ) by taking the average of the daily soil volumetric water contents from germination to flowering and calculating this as a proportion of the difference between field capacity and wilting point for that soil type.

The number of seeds produced per head is sampled from a log-normal distribution with mean=4.5779 and standard deviation=0.2337. The mean and standard deviation of this distribution are estimated from the data provided by Moss (1990). A proportion of this total seed production will be non-viable, this proportion is sampled from a normal distribution:  $\mathcal{N}(0.55, 0.126)$ , the mean and standard deviation are again estimated from the data provided by Moss (1990).

### 6.4.6 Seed Losses

The amount of seed lost is sampled from a the distribution: Lognormal( $-0.8070, 0.1303$ ), and seed survival in the soil follows the distribution:  $\mathcal{N}(0.3, 0.077)$ . The means and standard deviation of these distributions are estimated from data obtained by Moss (1990).

### 6.4.7 Seed Dispersal

We modelled both natural *A. myosuroides* seed dispersal and dispersal of seed by the combine and cultivation. The probability distribution for each dispersal process was calculated by numerical integration as:

$$P(m, n) = \frac{S^{(n-0.5)} S^{(m-0.5)}}{S^{(n-0.5)} S^{(m-0.5)}} \int \int f(x, y) dx dy \quad (6.25)$$

where  $S$  is the side length of the cell,  $P(m, n)$  is the probability of a seed falling into a cell at the distance from the source  $x = m, y = n$  and  $f(x, y)$  is the dispersal probability function.

The natural dispersal of *A. myosuroides* seed is assumed to be isotropic and to follow the rotated Gaussian distribution

$$f(x, y) = \frac{1}{2\pi\sigma^2} \exp \left[ -0.5 \left[ \left( \frac{x - \mu}{\sigma} \right)^2 + \left( \frac{y - \mu}{\sigma} \right)^2 \right] \right] \quad (6.26)$$

described by Paice *et al.* (1998). Each type of nearby cell is assessed in turn by integration as described above following the order indicated in Figure 6.6 until a total proportion of 0.999 has been accounted for. As was described by Paice *et al.* (1998), the mean ( $\mu$ ) of the distribution is set at 0 and the standard deviation ( $\sigma$ ) at 0.3. If any seeds remain these are dispersed to a randomly allocated cell to represent other sources of seed dispersal not accounted for here. The resulting list of proportions are stored and used throughout each yearly cycle of the model to move seeds from one cell to nearby cells

Dispersal by the combine and cultivation is anisotropic with seeds being dispersed



**Figure 6.6.** Numerical order of assessment of nearby squares for the dispersal of seeds from a plant in the centre square (labelled “1”). Cells with the same number all receive the same proportion of seed from the starting cell. If required, the pattern continues in the same manner expanding outwards.

in the direction of travel (Lutman *et al.*, 2002). In order to model the way in which seeds were moved by the combine, we considered two further Equations (6.27 and 6.28) defined by Paice *et al.* (1998), where  $x$  is the distance from the starting plant and  $c_t$  is the transition point between the Gaussian (Equation 6.27) and exponential (Equation 6.28) components.

$$z(x) = \frac{1}{\lambda\sqrt{2\pi}} \exp\left(-0.5\left(\frac{x-\varepsilon}{\lambda}\right)^2\right) \quad \text{for } x \leq c_t \quad (6.27)$$

$$z(x) = b \exp(-bx) \quad \text{for } x > c_t \quad (6.28)$$

However, to be able to use this function in the same way as described above for natural dispersal we need to be able to integrate the area under the curve. As this is a combination of two functions it does not integrate to 1 and so we used an exponentially modified Gaussian distribution instead (Equation 6.29) and estimated the parameters  $\gamma = 10/3$ ,  $\lambda = 0.1$  and  $\varepsilon = -0.15$  to best represent the distribution described by Paice *et al.* (1998).

$$f(x, y) = \frac{\gamma}{2} \exp\frac{\gamma}{2}(2\varepsilon + \gamma\lambda^2 - 2x) \operatorname{erfc}\left(\frac{+\gamma\lambda^2 - x}{\sqrt{2\lambda}}\right) \quad (6.29)$$

In this case the distribution is integrated and the area under the curve above each grid cell assessed in turn for a maximum of five grid cells in the direction opposite to the direction of travel and then towards the direction of travel until a total proportion of 0.999 is accounted for. Any remaining seeds are randomly allocated to a grid cell, in the direction of travel, up to a maximum dispersal distance of 20 m. The direction of travel is set up along the  $x$  axis of the grid from west to east for the first set of rows up to the width of the cultivator (40 m). It is then switched to travel east to west. The direction changes every time the number of rows reaches a multiple of the cultivator width.

For both natural dispersal and the seed movement by combine and cultivation, if seeds are to be moved into a cell that lies outside of the model arena the process is reflected off the arena boundary and back into the field. This simulates the idea that the modelled area is representative of a real field and boundaries are a source of seed (Marshall, 1989) and so rather than have seed loss at boundaries, any weeds present in margins could enter the cropped area.

#### 6.4.8 Vertical Movement of Seed in the Soil

Seeds are also moved vertically between the shallow and deep soil layers according to the type of cultivation used. In years when the cultivation type is set to “plough” a proportion of seeds from the shallow soil layer are buried into the deep soil layer drawn from a log-normal distribution with mean =  $-0.0515$  and standard deviation =  $0.0191$ , conversely some seeds are brought up to the shallow soil layer — this proportion is drawn from a log-normal distribution with mean =  $-1.0570$  and standard deviation =  $0.1199$ . For all other cultivation types there is no upward movement of seed (from the deep soil layer to the shallow soil layer). For tine cultivation at 10 cm the proportion of seeds that are buried (taken from the shallow soil layer and moved to the deep soil layer) is taken from the distribution  $\mathcal{N}(0.2, 0.051)$  and for tining at 20 cm the proportion is taken from the distribution  $\mathcal{N}(0.4, 0.101)$ . In years where a shallow cultivation is chosen (<5 cm tine) no seeds move vertically, in either direction. The parameters for these distributions are estimated from the data given by Moss (1990).

## 6.5 Model Validation

### 6.5.1 Patch Location

To validate the model, we simulated three fields for which *A. myosuroides* counts and all environmental inputs (soil texture, organic matter, pH, water, and topography) were available. The three fields were Harpenden, Redbourn and Haversham as detailed by Metcalfe *et al.* (2017c (Chapter 3)). As an initial investigation, we used the kriged maps of soil properties, which provides the best unbiased estimate at all unsampled locations. We kriged at a 1-m grid resolution and set our model grid-cell size to match this. As the model requires a rectangular grid input we kriged the data to the extent of the smallest rectangle that completely covers the whole field. We also input the day on which the gravimetric water content measurement was taken (Julian day). We simulated 40 years of growth starting with an initial seed bed of 10,000 seeds per cell, 20% of which were in the top soil layer. We chose three typical cultivation systems in use on arable land: (i) rotational cultivation with three years of tillage at <5 cm followed by one year using the plough, (ii) tillage at 10 cm, and (iii) tillage at <5 cm.

We took the output of the model only for years 11–40 from each simulation to allow for the location of patches to stabilise following the initial seeding at all locations. We recorded and mapped the average number of plants at each location in the field (1 m × 1 m grid cell) across these years and for 10 different simulations of the model (a total of 300 realisations of the field), we then compared these maps with the kriged distribution of *A. myosuroides* plants for that field. We calculated Pearson correlation coefficients between the density of seedlings in each cell and the kriged data from the field for each realisation of the field produced. We plotted a histogram of the resulting correlation coefficients for each cultivation type in each field to see the resulting distribution of correlations.

### 6.5.2 Scale-dependent Correlations

We wanted to see if the scale-dependent relationships found by Metcalfe *et al.*, (2017c (Chapter 3)) were an emergent property of the model. To do this we needed to simulate soil realistic of that found in the fields, but that maintained fine-scale variation which is lost in the kriged maps. We created the covariance matrix for each soil property in

each field from the covariance function corresponding to the variogram fitted to the soil data. To simplify the simulation we used the spherical model for the variogram in all cases. To simulate soil with realistic variation in soil properties, we used lower upper decomposition of the covariance matrix (Webster & Oliver, 2007, chapter 12). This simulates soil with realistic variation based on a vector of random numbers drawn from a normal distribution. In our case, however, we wanted to maintain the distribution of soil observed in the fields to see if the same distribution of *A. myosuroides* could be observed. To do this we conditioned the simulation to include our measured soil properties at the location where they were measured. The  $R$  conditioning data are transformed to standard normal form (denoted by the vector  $\mathbf{z}$ ) and the values at  $S$  unsampled positions are drawn independently at random from a standard normal distribution (vector  $\mathbf{g}$ ). To obtain the vector of conditionally simulated values ( $\mathbf{y}$ ) we use

$$\mathbf{y} = \begin{bmatrix} \mathbf{z}_R \\ \mathbf{L}_{SR}\mathbf{L}_{SS}^{-1} + \mathbf{L}_{RR}\mathbf{g}_S \end{bmatrix} \quad (6.30)$$

where  $\mathbf{L}$  is the lower triangular matrix obtained from the decomposition of the covariance matrix for the field. To reduce the computational intensity only data within the field boundary were simulated in this way. As the model requires a rectangular grid input we used the kriged data for all points lying outside of the field boundary up to the extent of the smallest rectangle that completely covers the whole field.

Following the simulation of the soil, we scaled the simulated values to match the mean and range of the original data values:

$$y = \frac{x - m}{s} \times s_{\text{obs}} + m_{\text{obs}} \quad (6.31)$$

where  $x$  is a simulated value,  $m$  and  $s$  are the mean and standard deviation respectively of all the simulated values for that soil property and  $m_{\text{obs}}$  and  $s_{\text{obs}}$  are the mean and standard deviation respectively for the observed data. Ideally we would have simulated all soil properties based on their covariances. However, due to the size of the field and the spatial scale of simulation this was not possible and so we performed a number of checks to prevent the simulation of impossible soil distributions. We checked that the scaled simulated values did not exceed realistic ranges for these soil properties: We limited clay, silt, organic matter, and soil moisture to being positive, and pH to

values between 1 and 14. Any simulations that fell outside of these acceptable ranges were discarded. We also checked that the simulated clay and silt values did not sum to values greater than 100 and so we paired simulations accordingly. We produced 35 suitable simulations for each soil property for the Harpenden and Haversham fields (the Redbourn field was too large to simulate in this way).

We simulated 40 years of growth starting with an initial seed bed of 10,000 seeds per cell, 20% of which were in the top soil layer. We implemented rotational cultivation with three years of tillage at <5 cm followed by one year using the plough as this is a typical recommendation to farmers for *A. myosuroides* control.

We took the output of the model only for years 11–40 from each simulation to allow for the location of patches to stabilise following the initial seeding at all locations. We extracted the number of *A. myosuroides* plants at each of the sampling locations from the original study (Metcalf *et al.*, 2017c (Chapter 3)) from the model output and did the same analysis of the nested sampling design as described by Metcalf *et al.* (2016 (Chapter 2)) to give scale-dependent correlation coefficients between the *A. myosuroides* counts and each soil property present in the model (clay, organic matter, pH and water) for each of the 1050 realisations of the field. We plotted a histogram to look at the frequency of these correlations across all 1050 realisations of the field given by the model and compared this distribution to the value obtained in the field data for each spatial scale and each soil property (Metcalf *et al.*, 2017c (Chapter 3)).

## 6.6 Results

### 6.6.1 Patch Location

The locations of the patches predicted by the model were broadly similar to those observed (Figure 6.7). At a coarse scale there are broad similarities between the distribution of *A. myosuroides* observed in the field and the predicted distributions from the model for all fields. In Harpenden, the rotational ploughing system led to very similar distributions, whereas the other two cultivation systems (10 cm tine, and <5 cm tine) showed much more uniform distributions across the field (Figure 6.7 a–d), this was also shown by the weaker correlations observed between the kriged *A. myosuroides* counts and the model predictions (Figure 6.8 a–c). For the field in Redbourn the high

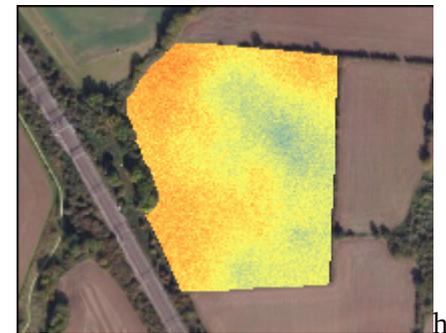
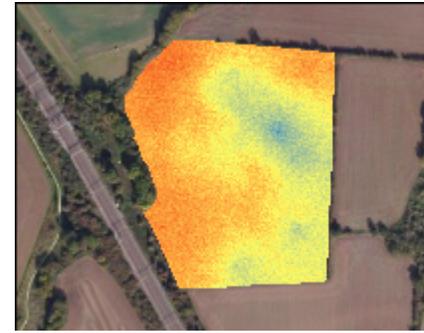
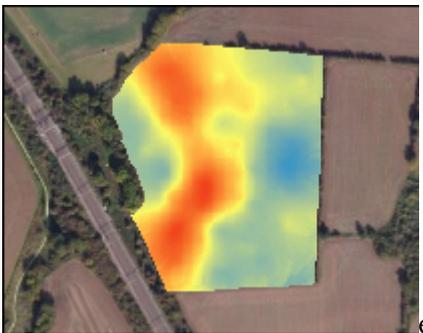
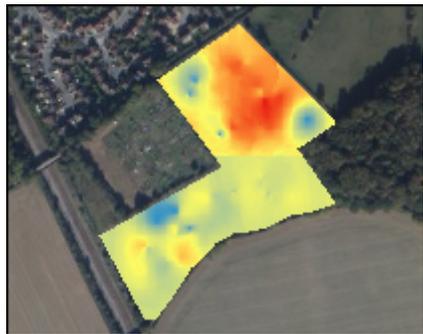
*A. myosuroides* counts in the eastern part of the field were reflected in the predictions, as were the low counts in the southern part of the field. However, in the west the observed and predicted distributions differ (Figure 6.7 i–l). Again, the strongest correlation between the kriged data and the model prediction we found was when we implemented the rotational ploughing cultivation system (Figure 6.8 g–i). Finally, in Haversham the western part of the field shows similar patch locations to those observed in the field (Figure 6.7 e–h, Figure 6.8 d–f). In all cases the predicted seedling densities are larger than were observed in the field and the patches more extensive.

Kriged log(Seedlings+0.1)

Rotational Plough

10 cm tine

<5 cm tine



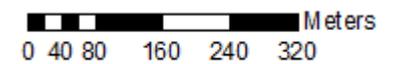
-2.303  5.784

3  7

7.8  8.6

8.5  9.1

Figure 6.7. Figure legend on page 176.



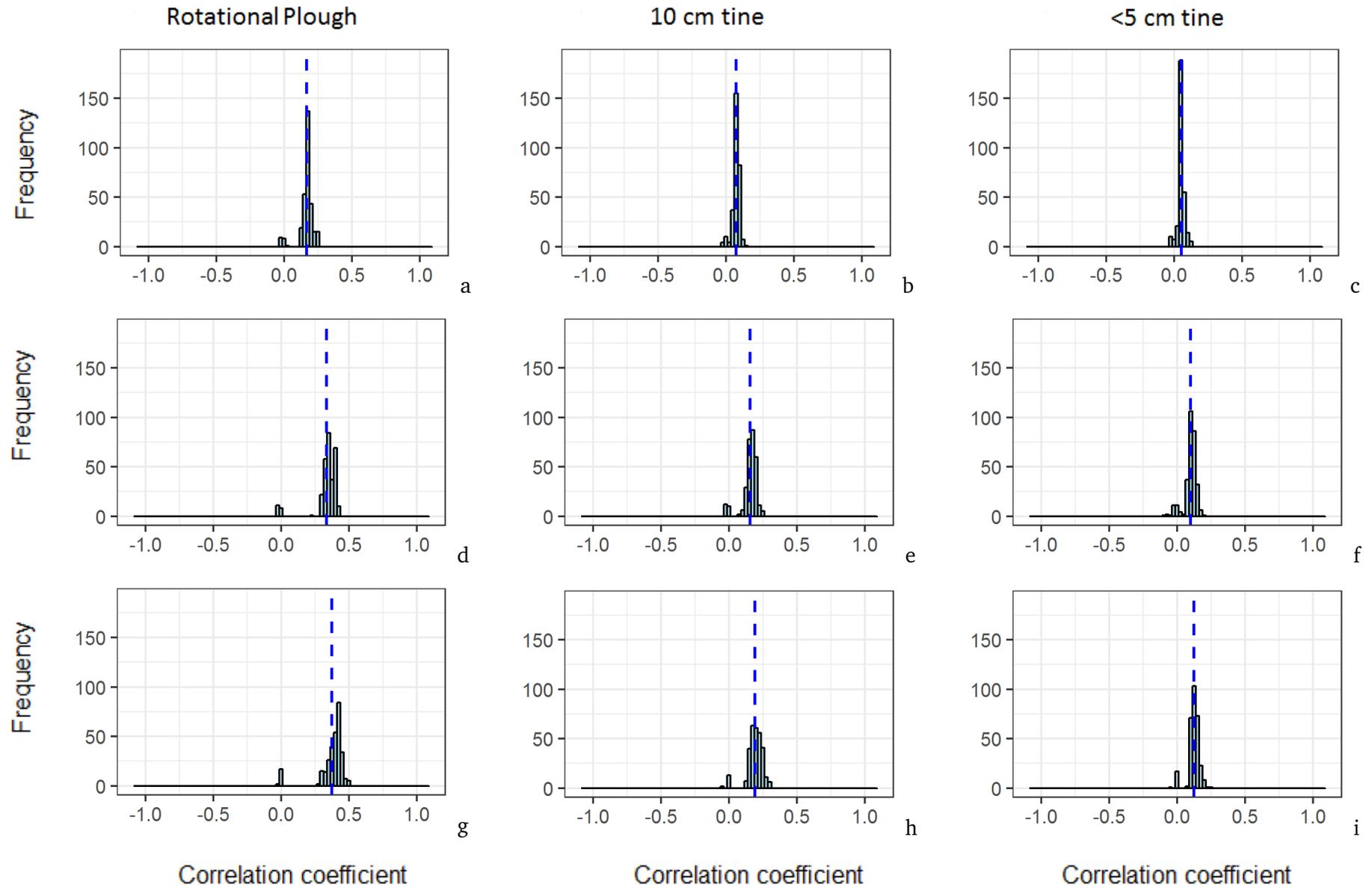


Figure 6.8. Figure legend on page 176.

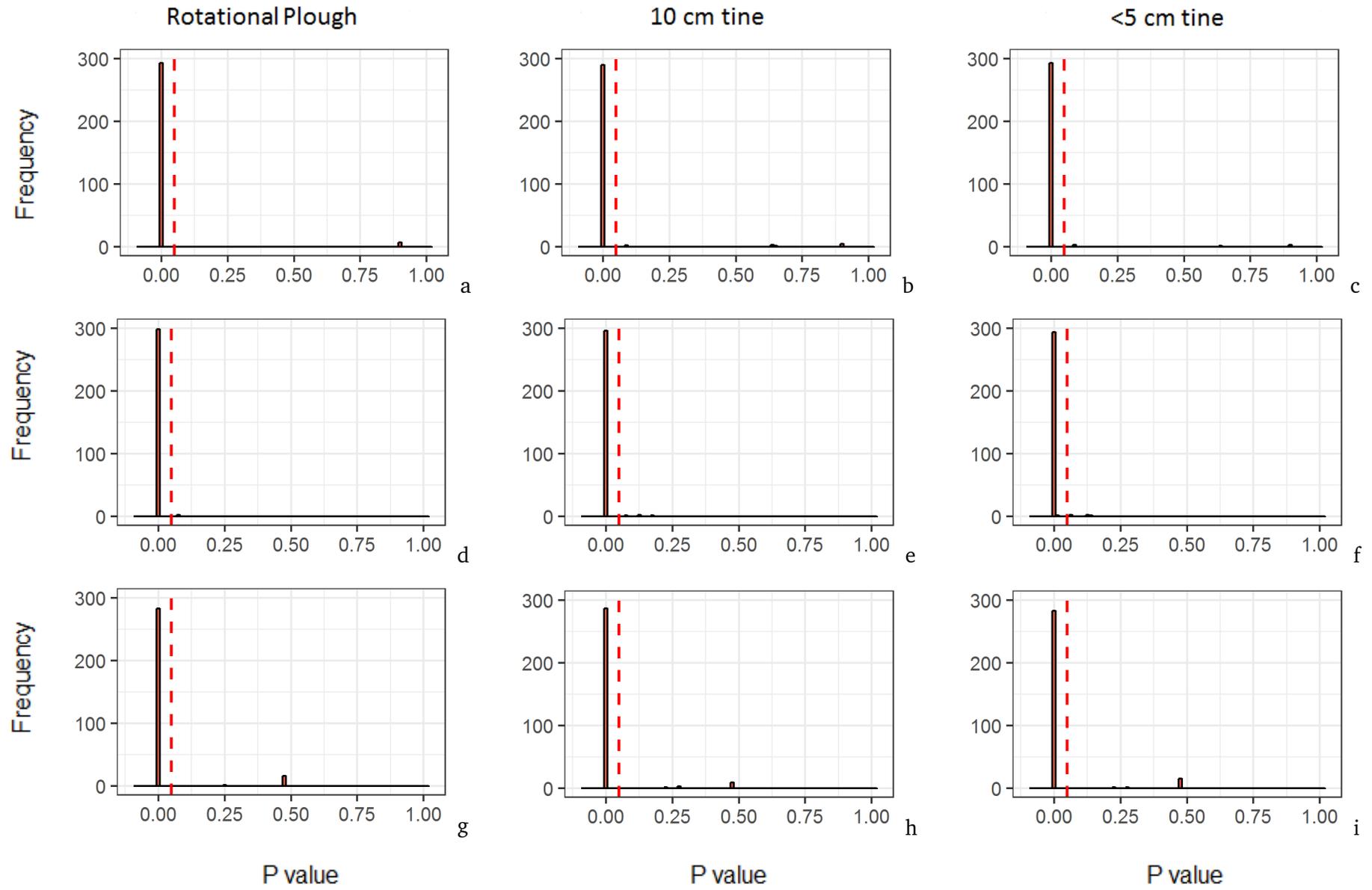


Figure 6.9. Figure legend on page 176.

**Figure 6.7.** (Figure on page 173.) Maps of Harpenden (top row: a–d), Haversham (middle row: e–h) and Redbourn (bottom row: i–l) showing the kriged log seedling counts (first column: a, e and i) and model outputs (columns 2–4: b–d, f–h, and j–l). Each model output shows the average log seedling density in each cell across 300 realisations of the field. The simulations in the second column (b, f, and j) are the output from the model simulations with rotational ploughing as the cultivation type — ploughing every fourth year with tining at <5 cm in the intermediate years. The simulations in the third column (c, g, and k) used 10 cm tining each year, and the simulations in the fourth column (d, h, and l) used <5 cm tining. Colour scales are maintained within columns and are applicable to each cultivation type separately.

**Figure 6.8.** (Figure on page 174.) Frequency distribution of correlation coefficients between model simulations and kriged log seedling counts for Harpenden (top row: a–c), Haversham (middle row: d–f) and Redbourn (bottom row: g–i). For each of the 300 realisations a correlation coefficient was calculated, the mean of these correlation coefficients is shown as a dashed line. The simulations in the first column (a, d, and g) are the output from the model simulations with rotational ploughing as the cultivation type — ploughing every fourth year with tining at <5 cm in the intermediate years. The simulations in the second column (b, e, and h) used 10 cm tining each year, and the simulations in the third column (c, f, and i) used <5 cm tining.

**Figure 6.9.** (Figure on page 175.) Frequency distribution of P values associated with correlation coefficients shown in Figure 6.8 between model simulations and kriged log seedling counts (bottom row: g–i). For each of the 300 realisations a correlation coefficient was calculated. Values to the left of the dotted line ( $P=0.05$ ) are statistically significant. The simulations in the first column (a, d, and g) are the output from the model simulations with rotational ploughing as the cultivation type—ploughing every fourth year with tining at <5 cm in the intermediate years. The simulations in the second column (b, e, and h) used 10 cm tining each year, and the simulations in the third column (c, f, and i) used <5 cm tining.

## 6.6.2 Scale-dependent Correlations

When we sampled the model output (with simulated soil) for the Harpenden and Haversham fields with the nested sampling design we observed the scale-dependent correlations between certain soil properties and the predicted *A. myosuroides* densities.

The scale-dependent correlations between *A. myosuroides* and clay were fairly consistent with those observed in the field by Metcalfe *et al.* (2017c (Chapter 3)). At coarse scales the model simulations largely resulted in large positive correlations (Figure 6.10 a and 6.11 a). For Harpenden, this was close to the observed correlation in the field of 0.85 and for Haversham the simulated correlations were often larger than that observed in the field (0.55), whereas at intermediate scales (Figure 6.10 b–d and 6.11 b–d) where the observed correlation in the field were weaker the prediction from the models were less conclusive with a range of correlation coefficients provided by the simulated data including both positive and negative correlations. At the finest scale included in the nested sampling all correlations between clay content and the simulated *A. myosuroides* seedling densities were small and often close to zero. This reflects the non-significant correlation of  $-0.04$  observed in the Harpenden field (A negative variance component was fitted in the Haversham field — this was not significantly different from zero— and so no correlation coefficient was calculated).

The results were similar for the relationships predicted between soil organic matter and *A. myosuroides* seedling densities with the model predicting large positive relationships with organic matter at coarse scales (Figure 6.10 f and 6.11 f), albeit often smaller than the correlation coefficients of 0.99 and 0.90 obtained from the field observations. There was no distinct pattern in the correlation coefficients at intermediate scales in Harpenden (Figure 6.10 g–i) and only small positive correlations at intermediate scales in Haversham (Figure 6.11 g–h), which were similar to the observed correlations of 0.22 and 0.62 at those scales. In both fields there were correlation coefficients close to zero at the finest scale between soil organic matter and *A. myosuroides* (Figure 6.10 j and 6.11 j).

When we consider pH and its relationship with *A. myosuroides* seedling densities in the Harpenden field we find a bimodal distribution in the correlation coefficients at coarse scales (Figure 6.10 k). This may be due to the way in which we incorporated soil pH in the implementation of the model as we applied a threshold below which

emergence levels would be increased (this chapter, Section 6.4.3). In some of our soil simulations this threshold would not be triggered and so the relationship with pH would be quite different in those simulations to the relationship observed when the threshold was reached. Again, at intermediate scales (Figure 6.10 l–n) there is no distinct pattern in the correlation coefficients and at fine scales all correlation coefficients are close to zero. In Haversham the REML model could not be fitted to the field data and so no comparison can be made with the simulated model outputs.

We found positive relationships with soil moisture content at the coarse-scale in the majority of simulations (Figure 6.10 p and 6.11 p). This result matched the significant positive correlation we found in the fields at this spatial scale. At intermediate scales (Figure 6.10 q–s and 6.11 q–s) The correlations between soil water content and *A. myosuroides* densities predicted by the model were less consistent with a range of correlations both positive and negative predicted by different model simulations. At the finest scale (Figure 6.10 t and 6.11 t) the relationship between soil water content and *A. myosuroides* seedling counts predicted by the model was often close to zero in both fields. However, at this fine scale our field observations gave quite large correlations and lay outside of the distribution of correlations predicted by our model.

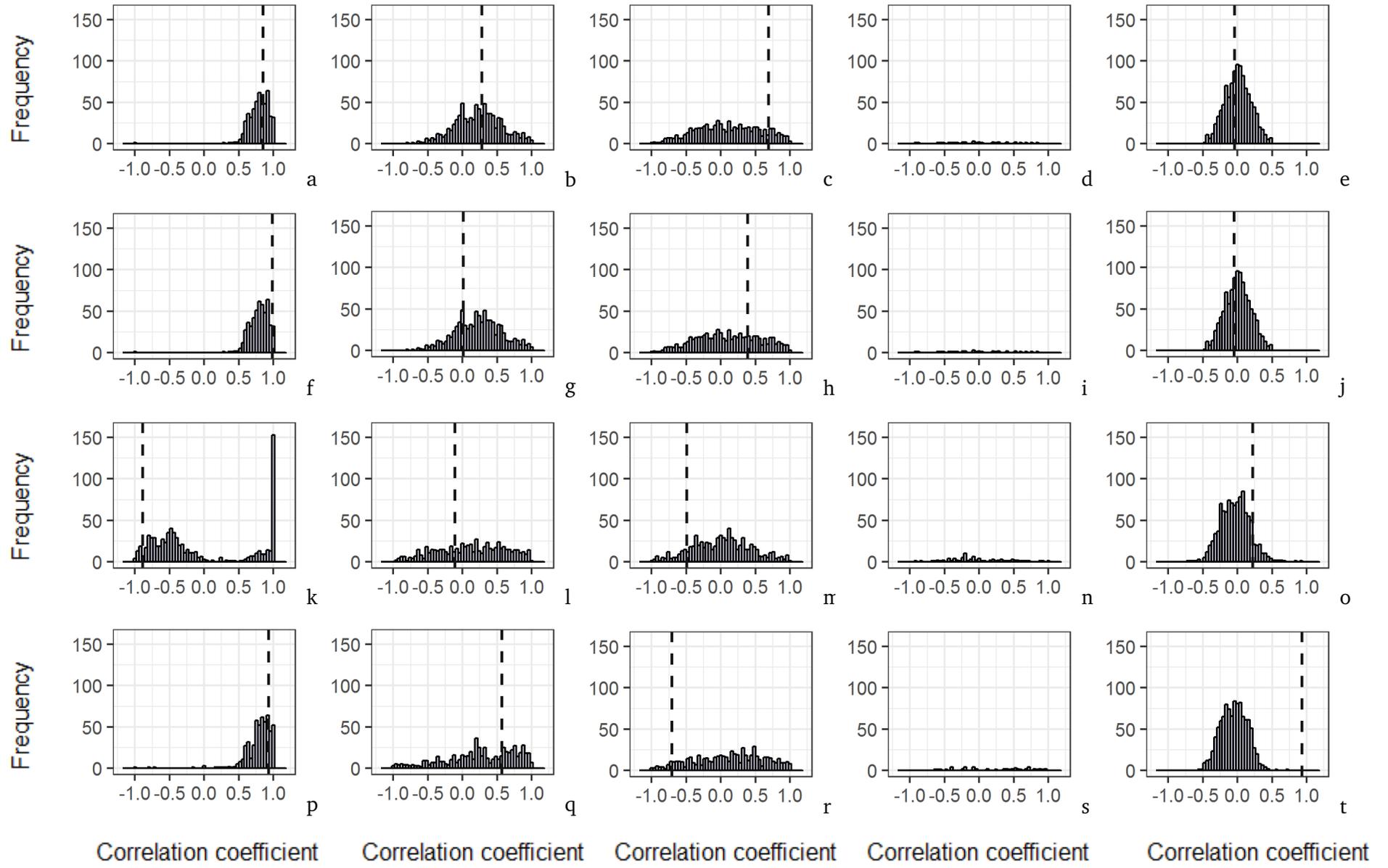


Figure 6.10. Figure legend on page 181.

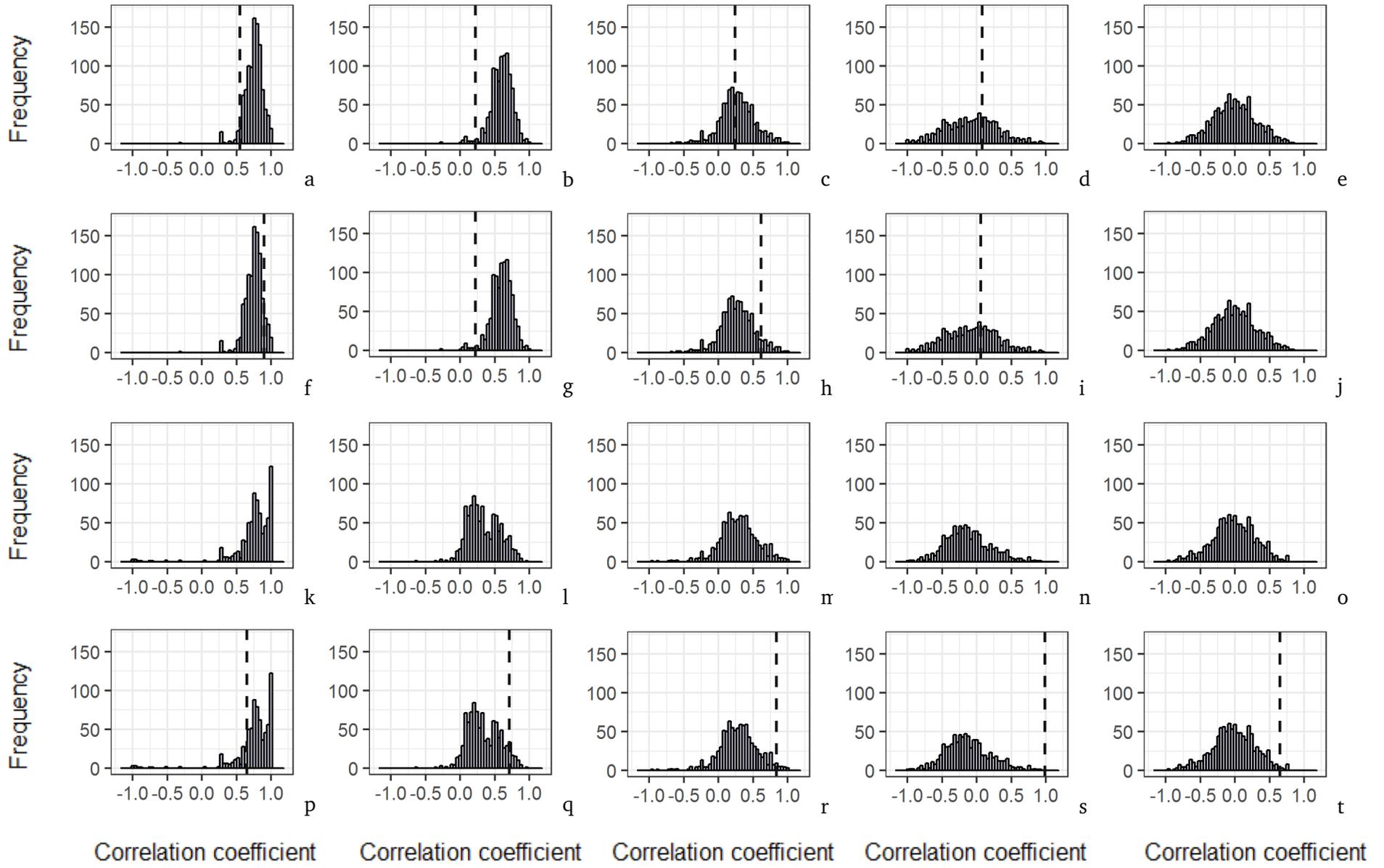


Figure 6.11. Figure legend on page 181.

**Figure 6.10.** (Figure on page 179.) Frequency distribution of scale-dependent correlation coefficients between the simulated number of *A. myosuroides* seedlings and simulated soil properties used as inputs into the model simulations for the field in Harpenden. The dotted line represents the observed scale-dependent correlation in the field (Chapter 3). The correlations shown are between *A. myosuroides* seedlings and the soil properties clay (a–e), soil organic matter (f–j), pH (k–o) and water (p–t) and for each soil property a range of spatial scales are considered ranging from coarse-scale in the first column to fine-scale in the last column: 50+ m (a, f, k, p), 20 m (b, g, l, q), 7.3 m (c, h, m, r), 2.7 m (d, i, n, s), and 1 m (e, j, o, t).

**Figure 6.11.** (Figure on page 180.) Frequency distribution of scale-dependent correlation coefficients between the simulated number of *A. myosuroides* seedlings and simulated soil properties used as inputs into the model simulations for the field in Haversham. The dotted line represents the observed scale-dependent correlation in the field (Chapter 3). The correlations shown are between *A. myosuroides* seedlings and the soil properties clay (a–e), soil organic matter (f–j), pH (k–o) and water (p–t) and for each soil property a range of spatial scales are considered ranging from coarse-scale in the first column to fine-scale in the last column: 50+ m (a, f, k, p), 20 m (b, g, l, q), 7.3 m (c, h, m, r), 2.7 m (d, i, n, s), and 1 m (e, j, o, t).

The predicted scale-dependent correlations between *A. myosuroides* heads and soil properties (Supplementary Figure S6.1 and S6.2) were very similar to those we found between *A. myosuroides* seedlings and soil properties (Figure 6.10 and 6.11) despite the observed correlations in the field often being weaker for heads than they were for seedlings (see Chapter 3).

## 6.7 Discussion

Here we show that by modifying the life-cycle of this species according to experimental data about how the life-cycle is affected by soil we can accurately predict the spatial population dynamics of the species within surveyed fields in commercial production of winter wheat. Our results support in-field studies (Lutman *et al.*, 2002; Murdoch *et al.*, 2014; Metcalfe *et al.*, 2017c (Chapter 3)) that show soil is an important determinant in

the within-field distribution of *A. myosuroides*.

Our results suggest that our model can provide a good prediction of the location of patches within fields. Irrespective of the cultivation type implemented in the model the correlation between the average *A. myosuroides* densities across 300 realisations and kriged soil properties were consistently strong and positive (Figures 6.7–6.9). This indicates the usefulness of this model in locating *A. myosuroides* vulnerable zones within fields. Seedling densities were quite different under the different cultivation types, yet all provided a good estimation of patch location. This supports the conclusions from Colbach *et al.*, (2000) that densities are often highly variable and so the prediction of densities is less accurate than the prediction of patch location. This means that it is possible to predict patch locations irrespective of the cultivation practices in place on a farm, making the model useful as a decision support tool as it is not necessary to provide all the information about cultivation history in order to locate weed vulnerable zones. As densities predicted here were often higher than those observed in the fields it makes this model a conservative tool for the implementation of site-specific management as we are likely to predict higher densities of *A. myosuroides* than are observed. Therefore we are more likely to suggest the need to spray an area that would not need such control measures than we are to avoid spraying an area that has an *A. myosuroides* problem. This goes some way to addressing the concerns of farmers that patch spraying is too risky as individuals might be missed and the seed return from those individuals is too great to counter any cost savings from the reduced herbicide input.

Strong coarse-scale relationships between soil properties and *A. myosuroides* distributions were an emergent property of our model. These matched those observed in-field. This is important as it is at these coarse scales that the in-field correlations were strongest (Metcalf *et al.*, 2016 and 2017c (Chapters 2 and 3)) and so it is important that our model corroborates these observations. In the application of site-specific weed management coarse-scales of 50+ m such as those where we observe these strong correlations are the most useful for management, as it is at these coarse scales that most farm machinery operates. As such, if we can input pre-existing or supplemented soil maps, already in use on farm for other site-specific management practices, then we should be able to predict the likelihood of parts of the field being vulnerable to *A. myosuroides* and so be able to develop maps for patch spraying based on the output of this model.

As with all models of weed population dynamics there are some limitations to this model. However these are necessary in order to keep the model simple enough to be functional whilst retaining enough detail to understand the system (Fernandez-Quintilla, 1988). Initially some of the limitations of the model come due to a lack of field data and are also under-represented in other models of *A. myosuroides* such as those by Moss (1990) and Colbach *et al.*, (2006a). These include the fate of seeds after shedding where we have included a certain amount of seed loss but this is an all encompassing figure, which includes germination, predation and decay. Similarly for other life-cycle processes where we only have information on the range and mean of field data such as seed production. These values are drawn stochastically from distributions with these parameters but remain unaffected by other factors and the value drawn for one process is independent of all other processes within the life-cycle. In our model we assume that the density of the crop and other weeds are uniform across the field and so interspecific competition is excluded other than to prevent any further germination once a crop canopy is established (this is uniform across the field). As we base this model on the premise that the field is a heterogeneous environment this may not be a correct assumption to make, however, it is an assumption that is also made in other models for patch spraying purposes (e.g. Paice *et al.*, 1998). In order to simplify the model we have divided the soil into two layers: a shallow layer from which seeds can germinate and a deep layer. However, in reality the soil is a continuum and there will be a gradient over which seeds can germinate at different rates. Finally, seed dispersal is only barochorous or by cultivation in our model. Both of these methods of dispersal are independent of other factors, yet it has been shown that there can be some influence of wind speed on seed dispersal of *A. myosuroides* (Colbach & Sache, 2001) and equally, seed movement in the soil can depend on soil properties (Benvenuti, 2007).

### 6.7.1 Conclusions

We have drawn together experimental data on the impact of soil properties on the life-cycle and management of this important agricultural species and through a modelling approach demonstrated the important role played by soil properties in determining the within-field distribution of *A. myosuroides*. We have also shown that scale-dependent correlations between *A. myosuroides* and soil properties observed in the field are an emergent property of this model. This could allow it to become an effective management

tool as the coarse-scale correlations, which are shown to be of the greatest importance, are the ones that have the most relevance to management. Seedling densities predicted in all simulations were higher than observed densities in the field, which is beneficial given the conservative nature of farmers as the model is likely to predict higher densities than are present in the field.

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## Chapter 7

# Discussion

Throughout this thesis my main objective was **to identify environmental determinants of *Alopecurus myosuroides* Huds. (black-grass) patch location and use these to define weed vulnerable zones.** An improved understanding of the relationships between *A. myosuroides* and the abiotic environment, in particular the soil, could better equip farmers and agronomists to manage this species in a more sustainable manner through site-specific weed management. In order to achieve this I have tested four main hypotheses through a combination of field work, pot experiments and modelling in Chapters 3–6 respectively, (Chapter 2 presented a new sampling methodology to address Hypothesis 1). In this chapter I discuss some of my main findings and their implications for UK farmers and agronomists as well as some possible directions for future work.

**Hypothesis 1: The within-field spatial distribution of *A. myosuroides* is associated with the spatial distribution of environmental variables at scales appropriate for management.**

Previous studies that have attempted to investigate the link between *A. myosuroides* patch location and soil properties have been limited in their scope because they only sample at a single scale (e.g. Dunker & Nordmeyer, 1999 and 2000; Lutman *et al.*, 2002). They each observed weak correlations, sometimes with contradictory results. Their failure to account for scale meant that finer scale variation obscured the strong coarse-scale relationships that link *A. myosuroides* and soil properties. I examined the scale-dependence of correlations between the distribution of *A. myosuroides* and various

abiotic variables using a novel nested sampling design (described in Chapter 2). This design allowed me to study scale-dependent correlations between weed distributions and environmental properties, and as such revealed the importance of the coarse-scale associations missed by these previous studies. Through the implementation of this novel sampling design in a case-study field (Harpenden, Chapter 2) I determined the strongest correlations between *A. myosuroides* and soil properties were at coarse scales (50+ m). I was also able to identify, in this field, the scales at which *A. myosuroides* showed the greatest amount of variation, and so could use this information to optimize the sampling design for use in subsequent fields. In this field I showed that there is scale-dependence in both the variation of *A. myosuroides* seedling counts and soil properties, demonstrating the importance of studying variation at several spatial scales. When I examined only the overall correlation between two variables, uncorrelated variation between the variables at finer scales obscured the scientifically interesting, and practically important relations exhibited at coarser scales. From this first investigation in Harpenden I preliminarily identified soil organic matter, texture, water, and pH as being associated with *A. myosuroides* seedlings, particularly at coarse scales.

I investigated these scale-dependent correlations between *A. myosuroides* counts and soil properties further by sampling in multiple fields across different growing seasons to investigate if any of the observed relationships found in the case-study field were consistent across fields and at what scale the strongest relations are observed (Chapter 3). I found that in different fields the soil properties show different amounts of variation and many of these properties can be correlatively linked with *A. myosuroides* distributions. Interestingly, it was often at the coarser scales studied (>50 m) that I found the strongest relationships, which implies a practical relevance to farmers. Most machinery currently available on farm operates at scales of 20 m or greater and so it is helpful to know that this is a relevant scale for management, although machinery with section and nozzle control, which allows patch spraying at finer resolutions is becoming more readily available. If patch spraying were to be implemented based on soil maps then it may only be necessary to map the soil at this coarse resolution, reducing the sampling effort required for mapping. The identification of these coarse scale relationships is also useful in the design of future sampling. As I showed in Chapter 2, nested sampling designs can be optimised based on knowledge of the scales at which variation occurs.

By considering five separate fields I was able to confirm that the observed relation-

ships between *A. myosuroides* counts and soil properties were somewhat consistent across fields and growing seasons indicating that the patterns I observed may be general. This generality allowed me to identify a suite of environmental properties including pH, soil moisture content and topography which could be built into a REML model to predict *A. myosuroides* patch locations. My work accords with the work of others (e.g. Wilson & Brain, 1991; Krohmann *et al.*, 2006) that the distribution of *A. myosuroides* can be patchy in fields growing winter wheat for commercial purposes. Incorporating this spatial autocorrelation in *A. myosuroides* counts into the statistical model also improved my prediction of *A. myosuroides* densities.

In addition to these results, which addressed Hypothesis 1, my work in Chapter 3 also ascertained that the distribution of seed heads in the summer is a contraction of the initial seedling patch. This highlights a problem associated with current methods of patch spraying. Where *A. myosuroides* heads are mapped in the summer to guide herbicide application of seedlings in the following season (Walter *et al.*, 2002). Even if buffer zones are applied this may not be sufficient to account for the contraction of the patch over the growing season as well as dispersal to new areas. If the contraction of patches is caused by the environment, then this does not pose a risk to the farmer. However, if the contraction of patches during the growing season is because of effective management measures in the intervening period then there is a risk the patches could expand again if those same measures are not implemented in the following season. I also demonstrated that the patches of heads are less accurately predicted from soil properties than seedlings. Whilst the real-time mapping of seedlings still remains the best option this is still very difficult to do and so the identification of weed vulnerable zones by soil properties will be an improvement on current methodologies as it will most accurately identify seedling patches, which are the target for the application of pre-emergence herbicides.

A particularly interesting observation to emerge from this work was that in fields where infestation was highest (Haversham) and particularly low (Ivinghoe and Radbrook) there were weaker correlations between *A. myosuroides* numbers and soil properties. This indicates that the relationship between *A. myosuroides* and soil properties identified here may depend on plant density. The weak relationships where plant densities were low might indicate that the patch may not have reached all areas suitable for growth. In these cases the identification and spraying of weed vulnerable zones

is a useful approach as a farmer will capture all *A. myosuroides* individuals. Whereas where densities were high we saw spill-over out of the optimal parts of the field. Seed production was so great in these fields that the likelihood of seed germinating and plants growing outside of their optimal environment was increased. This impresses the importance of effective management of *A. myosuroides* populations, as once plant densities become sufficiently large their control becomes increasingly difficult and in such fields where densities become so high that there may be spillover from identified weed vulnerable zones then more drastic control measures may be required and site-specific management of this kind is no longer useful.

These results collectively support Hypothesis 1: The within-field spatial distribution of *A. myosuroides* is associated with the spatial distribution of environmental variables at scales appropriate for management. Taking this a step further, the use of soil properties in the prediction of patch locations looks promising as it is fairly consistent across fields and seasons, particularly if we consider the incorporation of spatial autocorrelation in the prediction of seedling numbers. Where the predictive power of this statistical model is poorest seems to be in the prediction of areas with no *A. myosuroides* seedlings. However, this model is more likely to predict that there will be *A. myosuroides* present when there is none — making it a conservative approach in terms of risk and so more likely to be useful to farmers.

**Hypothesis 2: Soil organic matter, moisture and pH affect the life-cycle of *A. myosuroides* from germination to seed return.**

Through my field studies I determined that there were two main axes of variation in soil properties (Figure 3.3 in Chapter 3). The first of these axes corresponded to variation in soil organic matter, texture, and moisture, whilst the second axis was largely due to variation in pH. In order to elucidate the mechanisms and processes underlying the spatial variation in *A. myosuroides* observed in the field I investigated the effect of these two sources of soil variation on all aspects of the life-cycle of *A. myosuroides* from germination to seed return, through a series of pot experiments (Chapter 4).

The germination of *A. myosuroides* was found to be affected by both soil organic matter and moisture through a change in the rate of accumulation of hydrothermal time. Where there was increased water input, hydrothermal time was accumulated more

quickly and so germination occurred at a faster rate. I would have expected a similar increase in germination on soil with higher soil organic matter as the water holding capacity of such a soil would be higher and so hydrothermal time should accumulate more quickly. However, the results were somewhat contrary to this expectation; the medium organic matter soil allowed more seeds to germinate than the high organic matter soil. I believe this may be caused by mulching from the compost used to elevate the soil organic matter. Interestingly there was some evidence for an effect of soil pH on *A. myosuroides* germination with more seeds germinating where the soil pH was lower. The change in germination with pH may also be a result of the altered chemistry of the soil affecting water uptake.

I observed no effects of any of the soil properties tested on phenology, but plant height was affected by both soil organic matter and moisture in an interacting manner. In low water conditions plant height decreased with increasing organic matter whereas when water was plentiful plant height increased with organic matter. Increasing organic matter also increased the number of seeds produced. I also demonstrated that changing soil pH could affect the competitive balance between *A. myosuroides* and the wheat. This indicates that soil pH may have some influence on the location of *A. myosuroides* patches. It is likely this effect is related to the availability of nutrients at varying soil pH; for example, nitrogen, phosphorus, and potassium are all limited in availability in acid soil, whilst iron, zinc, and copper become limited in more alkaline soil (Brady, 1984). The contrasting rooting structure and function of *A. myosuroides* and wheat have been suggested as a possible reason for the current distribution of *A. myosuroides* in relation to variation in soil properties (Stratonovitch *et al.*, 2012). Through these experiments I showed that changing soil properties, particularly those which may alter the availability of resources including water and nutrients can change the growth rate of this plant and may also therefore affect the competitive balance. When I compared these results to my field observations (Chapter 3) I saw that it supported the conclusion that soil properties, including water, organic matter and pH may have some controlling influence over the within-field distribution of *A. myosuroides*.

The results from my pot experiments could potentially be translated into the development of management practices. For example, delayed drilling is a common method of cultural control. However, if the timing of germination can be affected by environmental processes then perhaps this needs to be taken into consideration when developing such

management programmes. Additionally, the difference in the optimum pH for wheat and *A. myosuroides* suggests that soil amendments to adjust the pH could make the environment less favourable to *A. myosuroides* but still optimal for wheat. The use of crop cultivars that are more competitive under particular field conditions could also be considered for fields with particularly low pH or high organic matter for example.

**Hypothesis 3: Soil organic matter affects the efficacy of flufenacet and pendimethalin against *A. myosuroides* and the ability of the weed to withstand sub-lethal doses of those herbicides.**

Organic matter in the soil can lead to adsorption of herbicide (Farenhorst, 2006) and different herbicides may be more or less adsorbed by organic matter, dependent on their physical and chemical properties (Nordmeyer, 2015). As pre-emergence herbicides are applied directly to the soil, it is particularly important to understand how varying soil properties within fields may be affecting their efficacy, as this may also, in part, determine the within-field distribution of this species. I investigated the effect of soil organic matter on the efficacy of two pre-emergence herbicides against *A. myosuroides* and whether soil organic matter plays a role in the resulting sub-lethal effects (Chapter 5).

My results showed that soil organic matter plays an important role in the control of *A. myosuroides* achieved by flufenacet and pendimethalin. I found that the ability of *A. myosuroides* to survive pre-emergence herbicide application was significantly affected by soil organic matter. Specifically, the placement of the curve on the dose axis is altered significantly depending on the levels of organic matter in the soil. Soil with a greater concentration of organic matter shifts the dose-response curve to the right meaning a higher dose of herbicide is required to achieve the same reduction in survival. However, the asymptotes of these dose-response curves remained the same indicating that given a high enough dose the same level of control can be achieved across all soil organic matter levels. Similarly, the size of the plants after six weeks was also greatly affected by soil organic matter with surviving plants grown in soil with high organic matter typically being larger than those grown in soil with less organic matter. This indicates that on higher organic matter soil, where pre-emergence herbicides are used for *A. myosuroides* control there are likely to be more survivors than on lower organic matter soil and those surviving individuals will be larger and so more likely to be able to compete well with the crop plants. I investigated this further using a crop competition model and found

that seed production was generally predicted to be higher on high organic matter soil and this was maintained across a wider range of doses than on low organic matter soil.

These results indicate the potential for altering dose rates of pre-emergence application according to soil organic matter to ensure a uniform level of control is achieved, or where control is poor on organic matter rich soil the application of post-emergence herbicides could be adjusted to compensate for the reduced control by the pre-emergence herbicides. Precision herbicide application per soil type is possible in the same way that patch spraying of weeds is conducted as many farmers have soil maps of their farms and the uptake of precision agriculture is advancing. So, in fields where there are within-field gradients of organic matter, it should be possible to adjust the application rate of the herbicide to account for this.

In the absence of competition, we found that plants surviving the application of pre-emergence herbicides show few sub-lethal effects of having received that dose. They produce the same amount of total biomass and seed, the seed they produce also shows similar viability to unsprayed plants, implying that plants adjust partitioning of resources such that fecundity is not compromised. In a crop-free environment this has no cost but would reduce competition when growing with a crop. In the absence of competition, on soil where control is poor I would expect little subsequent reduction in growth, and so any surviving plants will go on to produce as much seed as in an unsprayed situation. However, I also demonstrated through a modelling approach that in the presence of competition the reductions in plant size at an early stage would likely have further effects on seed production due to the asymmetric nature of competition. When plant densities are particularly high then density dependent effects may overshadow the sub-lethal effects of the herbicide. However, in the presence of competition when plant densities are much lower then these reductions in growth at an early stage can lead to substantial differences later in the growing season, yet these plants do still survive and go on to produce some seed, albeit not as much as in an unsprayed situation. This presents a further opportunity to exploit precision management techniques by increasing the crop seed rate in areas of high organic matter so as to compensate for the reduced herbicide efficacy.

This work supported the claims of others (Blumhorst *et al.*, 1990; Nordmeyer, 2015) that there are non-trivial effects of soil organic matter on pre-emergence herbicidal efficacy, even within the small range of organic matters typical of the UK arable landscape.

This raises the question about the suitability of claims made on herbicide labels to suggest they remain effective on soil with up to 10% organic matter. Even if this is the case, perhaps it needs to be considered that the optimal dose may change according to the level of organic matter in the soil. This may have strong implications for minimal- and no-tillage systems where the aim is to increase the levels of organic matter in the topsoil as this could mean decreased levels of control by pre-emergence herbicides despite their increased reliance on herbicide as they are unable to control the weeds using cultivation.

My results support Hypothesis 3: Soil organic matter affects the efficacy of flufenacet and pendimethalin against *A. myosuroides* and the ability of the weed to withstand sub-lethal doses of those herbicides. The results indicate that increasing soil organic matter would lead to decreased efficacy of both flufenacet and pendimethalin in the control of *A. myosuroides*. I expect that this is a result of adsorption of herbicide. The differences between the two herbicides could be because of different levels of adsorption, as was described by Nordmeyer (2015) for pendimethalin and chlortoluron.

The outcome of this hypothesis driven work on pre-emergence herbicide efficacy on soil with different levels of organic matter, together with the results concerning the life-cycle of the plant indicate that there are additive effects of increased fitness of the plant on high organic matter soil and reduced efficacy of pre-emergence plant protection products. Each of the processes I observed individually, for example the increased seed return or reduced herbicide efficacy with increasing soil organic matter, would not be sufficient to explain the aggregation of weeds in the field. However, as many of these processes act on the weeds in the same direction there is sufficient cause to believe that their additive effects would lead to an effect on weed population dynamics with increased numbers on organic matter rich, wet soil, with low pH.

**Hypothesis 4: The scale-dependent relationships between soil properties and the density of *A. myosuroides* observed in fields is an emergent property of the effect of soil on the various aspects of the soil properties on the weed's life-cycle.**

Building on previous work modelling *A. myosuroides* (Moss, 1990; Paice *et al.*, 1998; Colbach *et al.*, 2006) I developed a life-cycle model for *A. myosuroides* that incorporates natural dispersal as well as dispersal by cultivation (Chapter 6). I adjusted various aspects of the life-cycle according to soil properties based on the results of my investigations in Chapters 4 and 5. I tested if the model was able to replicate the distributions

of *A. myosuroides* observed in Chapter 3 and also if the scale dependent relationships between soil properties and the density of *A. myosuroides* observed in the field were an emergent property of the modelling process (Chapter 6).

Through modelling, I have combined the experimental data on the effects of soil properties on the life-cycle and management of this important agricultural species to demonstrate the role played by soil properties in determining the within-field distribution of *A. myosuroides*. The model I developed provides a good prediction of the location of patches within fields. However, predicted seedling densities are quite different under different simulated cultivation types. I have also shown that scale-dependent correlations between *A. myosuroides* and soil properties observed in the field are an emergent property of this model with strong coarse-scale relationships between soil properties and *A. myosuroides* distributions proving to be the most important.

These findings support my hypothesis that through incremental changes to the life-cycle of *A. myosuroides*, due to soil properties, the within-field distribution of this species can be predicted. This shows the importance of the role of soil properties in determining the within-field distribution of the species and also the need to consider the life-cycle in an holistic manner as it is not one process that determines the distribution but rather a series of incremental changes to its life-cycle each caused by an adjustment due to a given soil property. It is only when we consider these as a whole that we can predict the location of patches within fields.

By addressing these four hypotheses I have met my main objective, which was to identify environmental determinants of *A. myosuroides* patch location and use these to identify weed vulnerable zones. I have developed our understanding of the role played by abiotic factors in determining the location of *A. myosuroides* patches, both through observed patterns in the field and through a modelling approach whereby I took empirical relationships between soil properties and life history traits and modelled the effect of these relationships on the spatial dynamics of this species in a spatially heterogeneous simulated field.

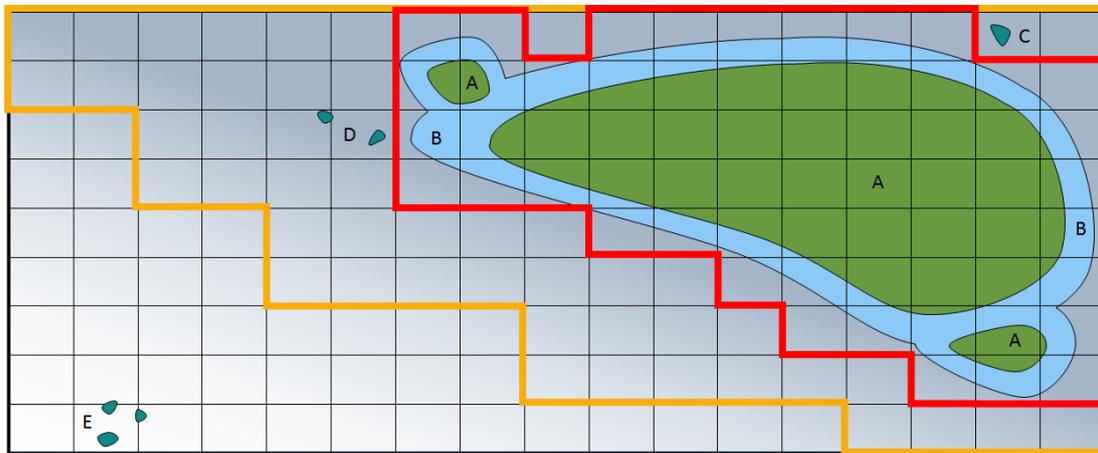
The emergent property of the model that coarse-scale correlations between *A. myosuroides* and soil properties are generally strongest is in accordance with my field data. This result is important in the application of site-specific weed management as these coarse scales of 50+ m are most useful for management, given that most farm machinery

operates at these scales. As such, if we can use pre-existing or supplemented soil maps, already in use on farm for other site-specific management practices, then we should be able to predict the likelihood of parts of the field being vulnerable to *A. myosuroides* and so be able to develop maps for patch spraying based on the output of this model.

As *A. myosuroides* seedling densities predicted by the model were often higher than those observed in the fields it makes this model a conservative tool for the implementation of site-specific management as it is likely to predict higher densities of *A. myosuroides* than are observed. Therefore we are more likely to suggest the need to spray an area that would not need such control measures than we are to avoid spraying an area that has an *A. myosuroides* problem. The statistical model described in Chapter 3 also has the benefit of being conservative in its prediction — it is more likely to predict the presence of *A. myosuroides* when it is absent than to indicate falsely a lack of *A. myosuroides* when it is there. These conservative predictions are beneficial if they were to be used in the creation of maps identifying weed vulnerable zones. The lack of uptake of patch spraying is often attributed to the inherent risk aversion of farmers when it comes to weed control. Current methods of patch spraying often fail to address this by only mapping heads in summer — a technique that we have shown to be unreliable in identifying the full extent of infestation within a field (Figure 7.1A). The addition of buffer zones around those patches (Figure 7.1B) goes some way to addressing this issue but is often not enough to convince farmers that the weed will still be controlled. Through the conservative predictions of our models we could identify areas of the field that are weed vulnerable zones and so capture any parts of the field that are susceptible to forming a new patch (Figure 7.1). As such, I suggest the most robust approach to site-specific weed control would be to combine weed maps with soil-based predictions of habitat suitability and weed vulnerable zones.

## 7.1 Recommendations for Further Research

My work has gone a long way towards identifying the soil properties responsible for determining the within-field distribution of *A. myosuroides*. However, there is still more work to do on determining the mechanistic response of the plant to those soil properties, and identifying how knowledge of soil properties can be used to locate weed vulnerable zones within fields.



**Figure 7.1.** Diagrammatic representation of the principles of patch spraying. Patch spraying often involves the mapping of weed patches within fields (A), either through manual surveying of heads or real-time detection. A buffer zone (B) is then drawn around these mapped patches to allow for the spread of the patch in the following season. The field is then divided into grids of a manageable size — often the width of the spray boom — and all grid cells that contain the patch and buffer zones will be sprayed (cells within the red line). This approach does not account for individuals dispersing outside of the buffer zones (C), being dragged long distances by the cultivator (D) or entering the field from the margin (E). If a suite of soil properties could be identified that are favourable to *A. myosuroides* (grey areas). Then we may be able to identify “weed vulnerable zones” and spray accordingly (cells within the yellow line). This presents a more conservative approach as a greater area of the field is sprayed, making it more appealing to farmers, yet still reducing the overall use of pesticide. It is likely that in this instance the seeds that fell outside of the original buffer zones, but are captured within the weed vulnerable zone, would have gone on to form a new patch (C and D). However, the seeds entering the field from the margin to land outside of the weed vulnerable zone (E) would not present a risk.

### **7.1.1 Improving the understanding of the within-field spatial distribution of *A. myosuroides***

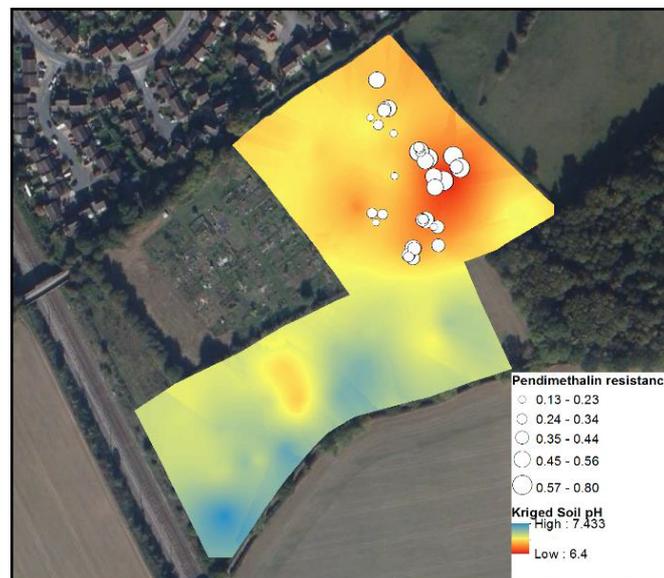
I believe it would be beneficial to extend my field studies (Chapter 3) to more fields. The fields I studied covered only a limited geographical area in south-east England, yet the range of *A. myosuroides* extends much further than this and a possible northward shift in its range is predicted with climate change (Stratonovitch *et al.*, 2012). By studying more fields encompassing the full extent of the geographical range of the species would allow the study of differing underlying soil types and levels of infestation. This would provide me with more data to make the statistical model for *A. myosuroides* seedling densities more robust and to confirm the selection of soil properties.

To extend my work looking at the direct effects of soil properties on the life-cycle of *A. myosuroides* it would be interesting to consider further experiments looking at additional soil properties and their effect on the life-cycle of *A. myosuroides* both in the presence and absence of competition. I would be particularly interested in extending the work from Chapter 4 to look at a greater range of soil organic matter contents and soil pH as these results provided some insight into the role of these soil properties in determining the within-field distribution of this species, but more detailed experiments would allow a better understanding of the mechanisms underlying those relationships. Similarly, my work looking at pre-emergence herbicides and soil organic matter in Chapter 5 highlights an opportunity for further research into the efficacy of other chemical control methods on different soil types and the role this plays in determining the within-field distribution of *A. myosuroides*.

### **7.1.2 Within-field spatial patterns of herbicide resistance**

Throughout this thesis I have focussed on the spatial distribution of *A. myosuroides*. This species is particularly problematic in the UK, largely because of its evolving resistance to herbicides. Whilst herbicide resistance is an important part of the narrative surrounding the control of this agricultural weed it has not been central to my objectives regarding its spatial distribution. It would nevertheless be interesting to combine the work presented in this thesis with the study of herbicide resistance by considering the effect of the local environment on the evolution and management of herbicide resistance.

It would be interesting to consider the herbicide resistance status of the fields studied in Chapters 2 and 3 as it might be that in fields with high levels of herbicide resistance the relationship with soil properties is different to that observed in fields with susceptible populations. Initial work indicates that some of the same soil properties that I found to be important in determining the within-field distribution of *A. myosuroides*, namely soil texture, organic matter and pH, can explain variance in the level of susceptibility to some herbicides (Figure 7.2); although it is unclear from these preliminary data the causality of this relationship. In order to investigate this further it would be possible to collect seed from all field sites and test their resistance status to see if there is spatial correlation with soil properties. It would also be interesting to run selection experiments on different soil types where plants are exposed to a range of herbicides to see if the evolution of resistance is accelerated on any particular soil type.



**Figure 7.2.** Results of resistance assay to pendimethalin (methods according to Moss, 2000) on seed sampled from the same quadrats as detailed in Chapter 2 in the Harpenden field. Resistance is focussed on the centres of high population density (compare Figure 2.5 in Chapter 2) associated with the parts of the field with lower pH. However, the mechanisms underpinning these patterns are unclear in terms of the interplay of evolutionary and ecological processes.

### 7.1.3 Development of the mechanistic model to identify weed vulnerable zones

The modelling component of my work detailed in Chapter 6 could also be developed further by investigating the effect of different cultural control practices in addition to the cultivation systems investigated here. It would be interesting to incorporate aspects of inter-specific competition into the model, as it is currently assumed to be uniform across the field. If I could incorporate the effect of the soil on the crop as well as the weed it may be possible to gain further insight into the mechanisms controlling the spatial distribution of the weed. It would also be interesting to implement different site-specific management programs within the model to determine the optimal means by which to implement these in the field together with the economics associated with each weed management program. As part of this it would also be useful to determine if seasonal variations in patch size are captured within the weed vulnerable zones predicted by the model.

In order, to make the model more useful in terms of its application in site-specific management it would be necessary to try and reduce the overall size of the model allowing it to process fields quickly and therefore be potentially of use on farm. This could be achieved through sensitivity analyses to determine which components of the model are most important in determining the output. The implementation of the model on farms could also be made more coherent by the development of simple algorithms allowing the input of existing soil maps available on farm in order to use these to identify weed vulnerable zones.

As I found that it is often at the coarse scale that the strongest relationships between *A. myosuroides* and soil properties are found, it could be possible to use the coarse-scale soil maps already in use on farms as inputs to the model. However in order to test the usefulness of these it would be necessary to verify the model at this scale. This could be done by kriging the soil properties for the fields investigated here at a much coarser resolution and using these maps as the input for the model and then seeing if the resulting output correlates with *A. myosuroides* densities kriged at the same resolution.

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# Modelling the Spatial Variation in *Alopecurus myosuroides* for Precision Weed Management

## Supplementary Material

Submission of thesis for the degree of PhD in Agriculture

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# Supplementary Material: Chapter 3

## — Defining the Habitat Niche of Black-grass (*Alopecurus myosuroides*) at the Field Scale.

**Table S3.1.** Terms selected in a regression type analysis using REML to predict *A. myosuroides* head densities from soil properties. The non-spatial model has only field location as a random effect, whereas the spatial model allows the estimation of a variogram as a random effect. Here a spherical variogram with a nugget of 2.470, range of 122.3 m and a sill of 1.136 was fitted.

Term	Effect	S.E.
<i>Non-spatial model</i>		
Constant	-0.8577	1.33253
Log(clay:sand)	2.292	0.4448
Log(silt:sand)	-1.998	0.5245
Soil organic matter	0.7466	0.20514
Gravimetric water content top 10 cm	0.3269	0.08080
<i>Spatial model</i>		
Constant	-1.023	0.3454
Phosphorus	-0.0451	0.019264
Gravimetric water content top 10 cm	0.1609	0.07105

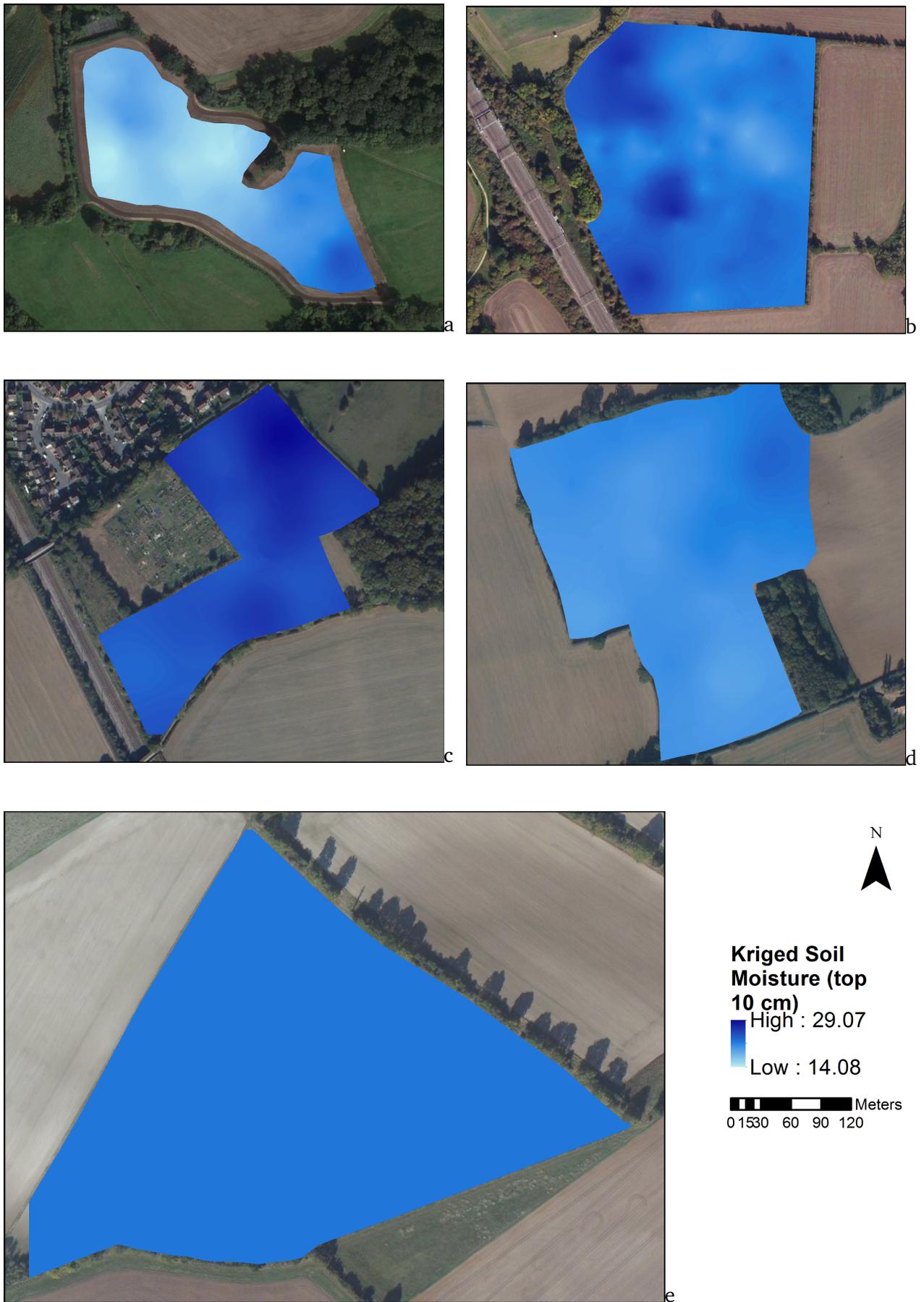


Figure S3.1. Figure legend on page 227.

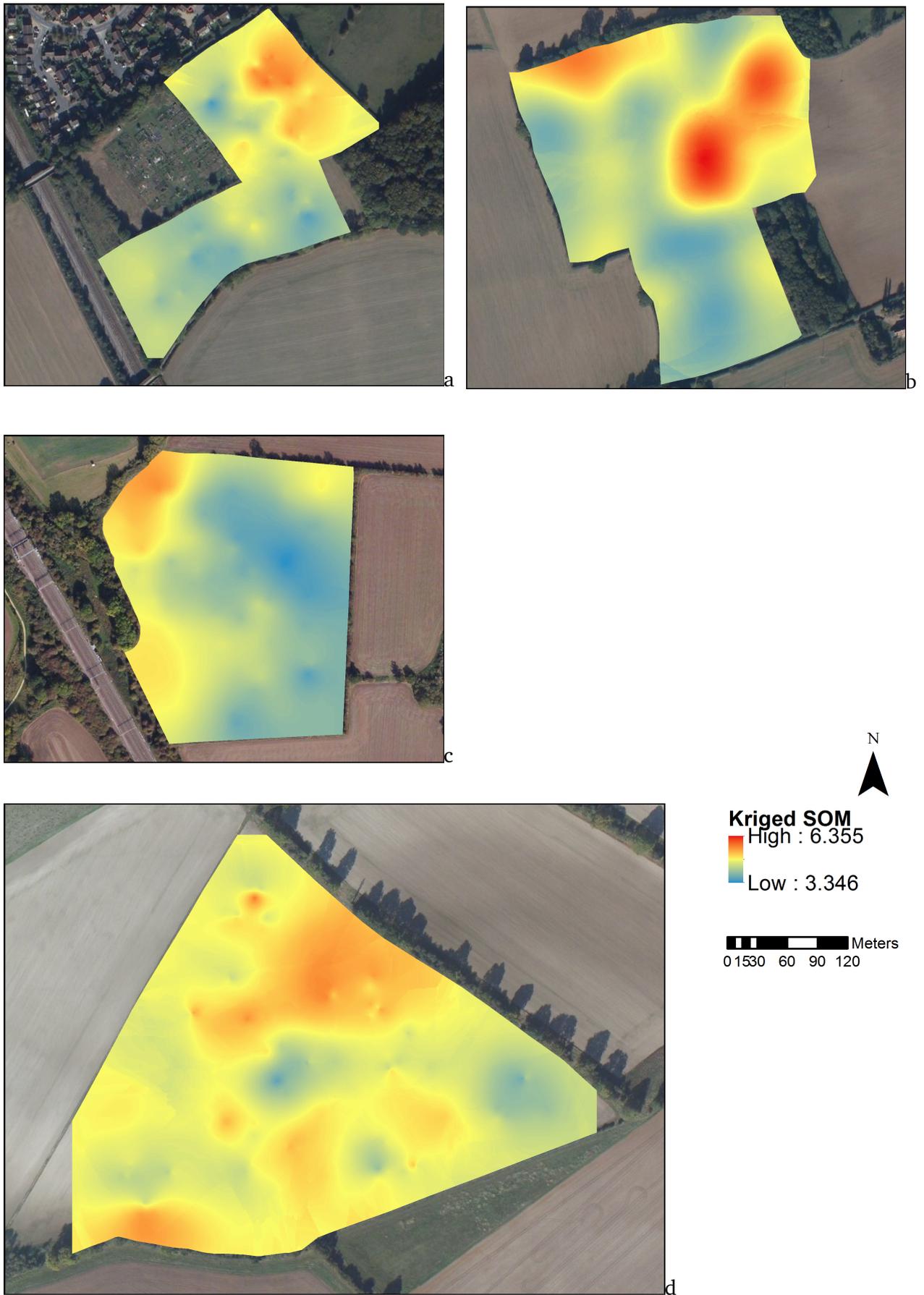


Figure S3.2. Figure legend on page 227.

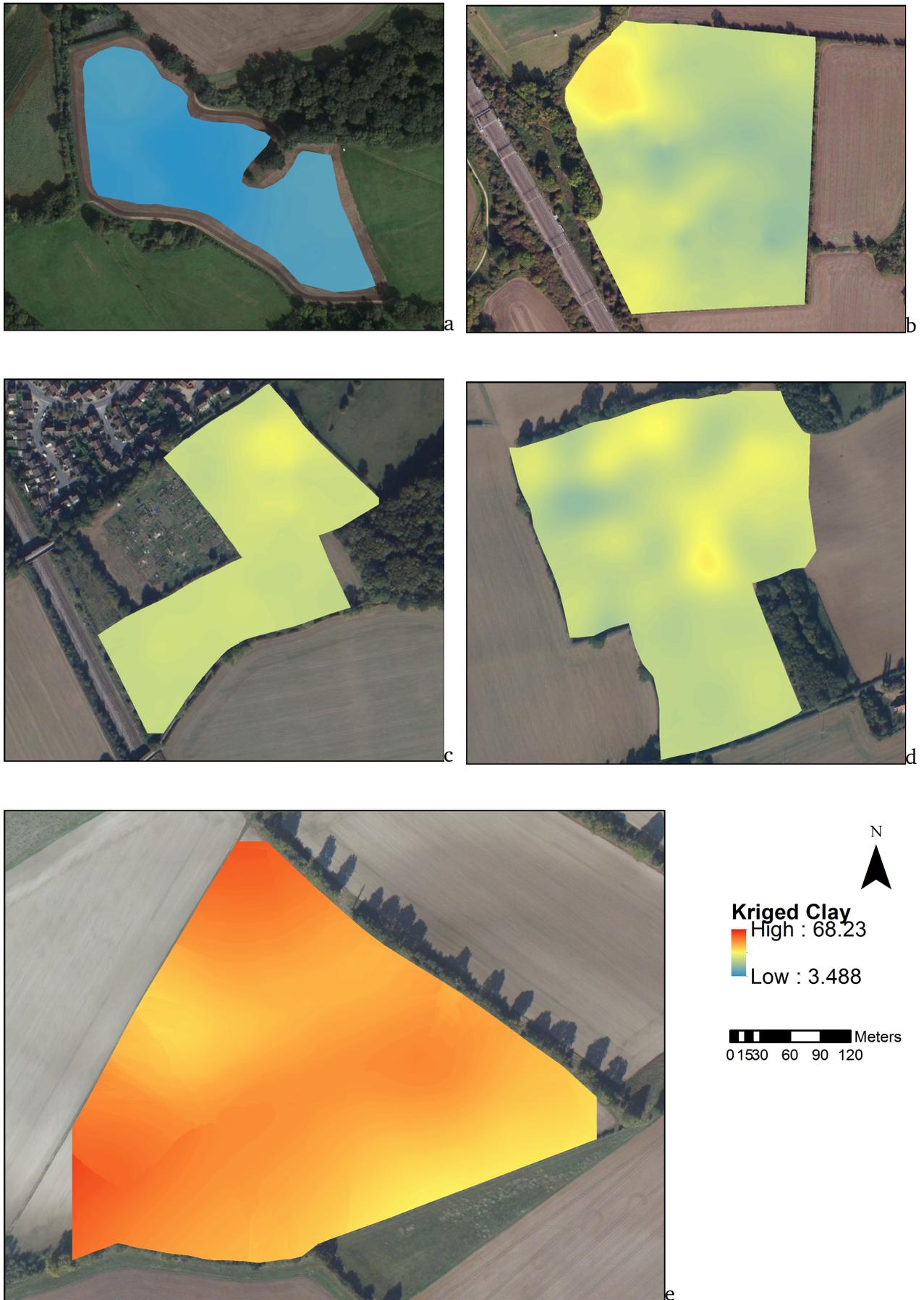


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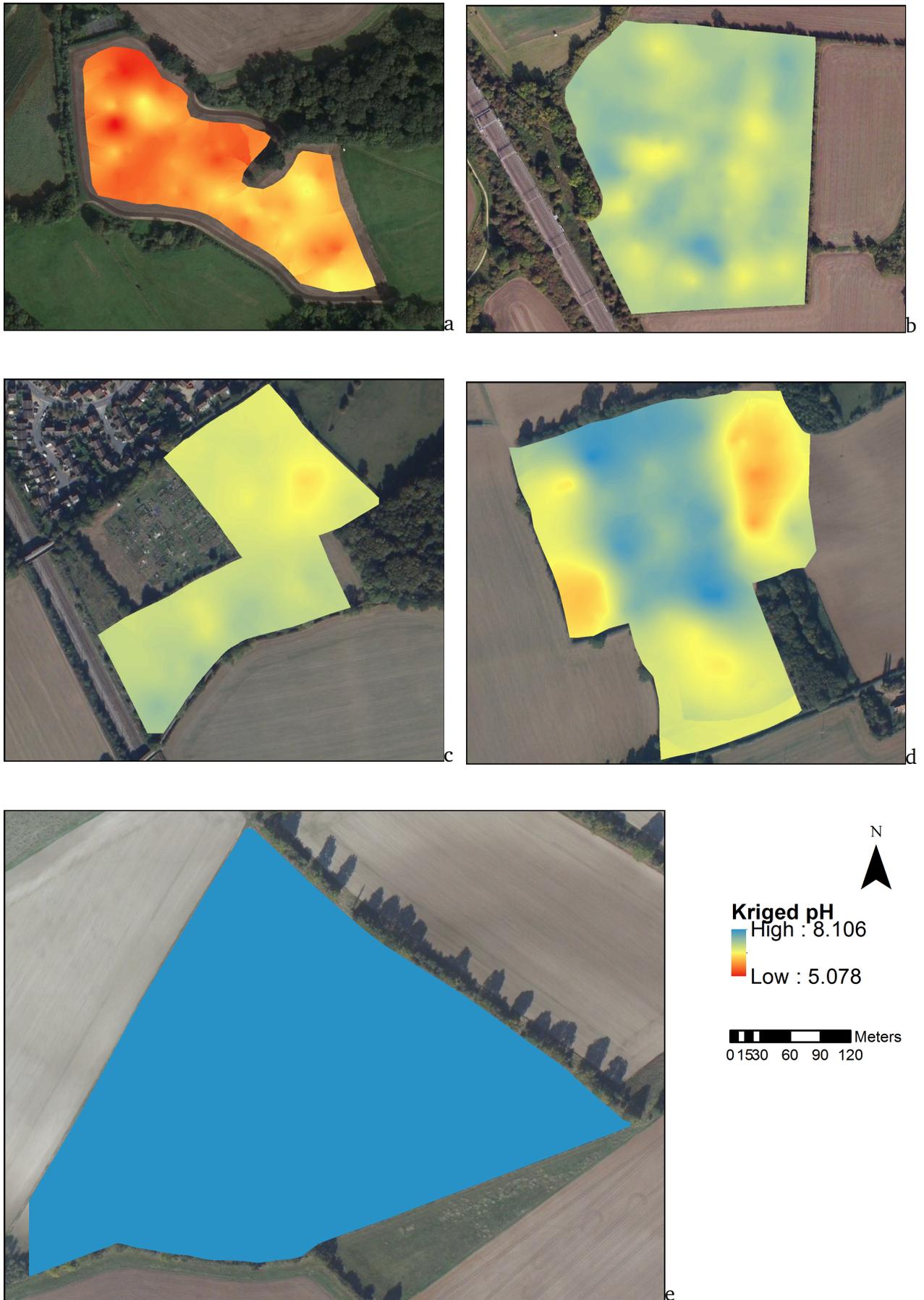


Figure S3.4. Figure legend on page 227.

**Figure S3.1.** (Figure on page 223.) Maps showing the kriged soil moisture content (0–10 cm) in each of the five fields (a) Radbrook, (b) Haversham, (c) Harpenden, (d) Redbourn, and (e) Ivinghoe, soil moisture is gravimetric in all cases except Radbrook where the volumetric moisture content is shown. The kriging was conducted using ordinary kriging based on the variogram fitted for that field.

**Figure S3.2.** (Figure on page 224.) Maps showing the kriged soil clay content in the four fields where it was measured: (a) Harpenden, (b) Redbourn, (c) Haversham, and (d) Ivinghoe. The kriging was conducted using ordinary kriging based on the variogram fitted for that field.

**Figure S3.3.** (Figure on page 225.) Maps showing the kriged soil clay content in each of the five fields (a) Radbrook, (b) Haversham, (c) Harpenden, (d) Redbourn, and (e) Ivinghoe. The kriging was conducted using ordinary kriging based on the variogram fitted for that field.

**Figure S3.4.** (Figure on page 226.) Maps showing the kriged soil pH in each of the five fields (a) Radbrook, (b) Haversham, (c) Harpenden, (d) Redbourn, and (e) Ivinghoe. The kriging was conducted using ordinary kriging based on the variogram fitted for that field.

# Supplementary Material: Chapter 4

## —The Effect of the Abiotic Environment on the Life-Cycle of Black-grass (*Alopecurus myosuroides*)

**Table S4.1.** ANOVA table for the total number of seeds germinating in Experiment 1, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	186.5	21.2	0.22	
Block.*Units* stratum					
Soil	2	2659.0	1329.5	9.25	<0.001
Water	1	9181.9	9181.9	63.91	<0.001
Soil.Water	2	283.9	141.9	0.99	0.384
Residual	30	4310.4	143.7		
Total	41	16621.6			

**Table S4.2.** Non-linear regression analysis to fit a Gompertz curve to germination data collected in Experiment 1, Chapter 4.

Source	d.f.	s.s.	m.s.	v.r.	F pr.
Single curve					
Regression	3	1100485	366828.2	1847.89	<0.001
Residual	669	132804	198.5		
Total	672	1233289	1835.3		
Separate Curve for each treatment					
Regression	18	1176830	65379.43	757.33	<0.001
Residual	654	556459	86.33		
Total	672	1233289	1835.25		
Change	-15	-76345	5089.68	58.96	<0.001

**Table S4.3.** ANOVA table for the Julian day of first flowering in Experiment 1, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	352.62	58.77	2.37	
Block.*Units* stratum					
Soil	2	28.76	14.38	0.58	0.567
Water	1	34.38	34.38	1.38	0.249
Soil.Water	2	0.76	0.38	0.02	0.985
Residual	30	745.10	24.84		
Total	41	1161.62			

**Table S4.4.** ANOVA table for the height of the plants at maturity in Experiment 1, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	729.7	121.6	1.08	
Block.*Units* stratum					
Soil	2	190.6	95.3	0.85	0.438
Water	1	2407.7	2407.7	21.45	<0.001
Soil.Water	2	2186.1	1093.1	9.74	<0.001
Residual	30	3367.2	112.2		
Total	41	8881.3			

**Table S4.5.** ANOVA table for the number of seed heads per plant at maturity in Experiment 1, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	15332	2555	1.58	
Block.*Units* stratum					
Soil	2	50297	25149	15.54	<0.001
Water	1	3659	3659	2.26	0.143
Soil.Water	2	5372	2686	1.66	0.207
Residual	30	48557	1619		
Total	41	123217			

**Table S4.6.** ANOVA table for the total dry weight of seed heads at maturity in Experiment 1, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	29.461	4.910	0.72	
Block.*Units* stratum					
Soil	2	40.292	20.146	2.95	0.068
Water	1	35.492	35.492	5.19	0.030
Soil.Water	2	4.878	2.439	0.36	0.703
Residual	30	205.190	6.840		
Total	41	315.313			

**Table S4.7.** ANOVA table for the total dry weight of seed heads at maturity in Experiment 1, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	141.09	23.52	0.55	
Block.*Units* stratum					
Soil	2	2732.30	1366.15	32.15	<0.001
Water	1	1.64	1.64	0.04	0.846
Soil.Water	2	32.32	16.16	0.38	0.687
Residual	30	1274.60	42.49		
Total	41	4181.95			

**Table S4.8.** ANOVA table for the total dry weight of seed heads at maturity in Experiment 1, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	239.95	39.99	0.72	
Block.*Units* stratum					
Soil	2	3273.33	1636.66	29.40	<0.001
Water	1	52.39	52.39	0.94	0.340
Soil.Water	2	48.66	24.33	0.44	0.650
Residual	30	1670.21	55.67		
Total	41	5284.54			

**Table S4.9.** ANOVA table for the total number of seeds germinating in Experiment 2, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	1570.7	261.8	2.14	
Block.*Units* stratum					
pH	1	94.5	94.5	0.77	0.385
Residual	34	4151.3	122.1		
Total	41	5816.5			

**Table S4.10.** Non-linear regression analysis to fit a Gompertz curve to germination data collected in Experiment 1, Chapter 4.

Source	d.f.	s.s.	m.s.	v.r.	F pr.
Single curve					
Regression	3	211852	70617.5	628.00	<0.001
Residual	333	37446	112.4		
Total	336	249298	742.0		
Separate Curve for each treatment					
Regression	6	212689	35448.1	319.53	<0.001
Residual	330	36609	110.9		
Total	336	249298	742.0		
Change	-3	-836	278.8	2.51	0.058

**Table S4.11.** ANOVA table for the Julian day of flowering in Experiment 3, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	1032.4	172.1	1.27	
Block.*Units* stratum					
pH	1	12.1	12.1	0.09	0.767
Competition	1	66.5	66.5	0.49	0.489
pH.Competition	1	4.6	4.6	0.03	0.856
Competition.SpeciesComp	1	404.3	404.3	2.98	0.094
Competition.SpeciesNoComp	1	100.3	100.3	0.74	0.396
pH.SpeciesComp	1	1.1	1.1	0.01	0.928
pH.SpeciesNoComp	1	26.0	26.0	0.19	0.664
Residual	34	4617.3	135.8		
Total	47	5994.8			

**Table S4.12.** ANOVA table for the height of plants in Experiment 3, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	1132.7	188.8	1.21	
Block.*Units* stratum					
pH	1	595.7	595.7	3.83	0.060
Competition	1	152.5	152.5	0.98	0.330
pH.Competition	1	0.4	0.4	0.00	0.961
Competition.SpeciesComp	1	462.1	462.1	2.97	0.095
Competition.SpeciesNoComp	1	108.1	108.1	0.69	0.411
pH.SpeciesComp	1	166.4	166.4	1.07	0.309
pH.SpeciesNoComp	1	60.0	60.0	0.39	0.539
Residual	31	4826.5	155.7		
Total	44	7007.9			

**Table S4.13.** ANOVA table for the number of seed heads in Experiment 3, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	39881	6647	2.15	
Block.*Units* stratum					
pH	1	596	596	0.19	0.663
Competition	1	21396	21396	6.92	0.013
pH.Competition	1	1200	1200	0.39	0.537
Competition.SpeciesComp	1	1257	1257	0.41	0.528
Competition.SpeciesNoComp	1	57876	57876	18.71	<0.001
pH.SpeciesComp	1	448	448	0.14	0.706
pH.SpeciesNoComp	1	472	472	0.15	0.698
Residual	34	105156	3093		
Total	47	220792			

**Table S4.14.** ANOVA table for the dryweight of seed heads in Experiment 3, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	3590	598	0.59	
Block.*Units* stratum					
pH	1	1400	1400	1.38	0.248
Competition	1	4	4	0.00	0.951
pH.Competition	1	695	695	0.69	0.413
Competition.SpeciesComp	1	1736	1736	1.71	0.200
Competition.SpeciesNoComp	1	83	83	0.08	0.776
pH.SpeciesComp	1	58	58	0.06	0.812
pH.SpeciesNoComp	1	62	62	0.06	0.806
Residual	33	33440	1013		
Total	46	39886			

**Table S4.15.** ANOVA table for the total plant dryweight in Experiment 3, Chapter 4.

Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	6	6844	1147	0.38	
Block.*Units* stratum					
pH	1	7726	7726	2.54	0.121
Competition	1	1423	1423	0.47	0.499
pH.Competition	1	916	916	0.30	0.587
Competition.SpeciesComp	1	3800	3800	1.25	0.272
Competition.SpeciesNoComp	1	16	16	0.01	0.943
pH.SpeciesComp	1	114	114	0.04	0.848
pH.SpeciesNoComp	1	8209	8209	2.70	0.110
Residual	33	100435	3043		
Total	46	123477			

**Table S4.16.** ANOVA table for relative biomass of plants when grown in competition to when grown in isolation in Experiment 3, Chapter 4.

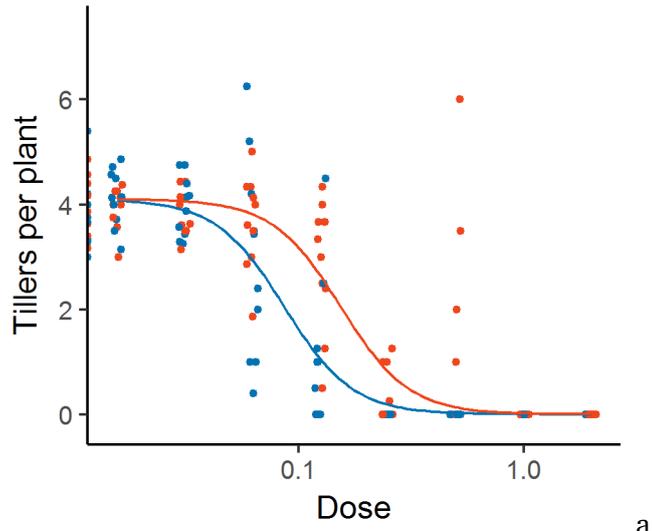
Source of Variation	d.f.	s.s.	m.s.	v.r.	F pr.
Block stratum	5	0.3811	0.0762	0.62	
Block.*Units* stratum					
pH	1	0.0403	0.0403	0.33	0.577
Species	1	1.1947	1.1947	9.78	0.009
pH.Species	1	0.4113	0.4113	3.37	0.091
Residual	12	1.4660	0.1222		
Total	20	3.2434			

# Supplementary Material: Chapter 5

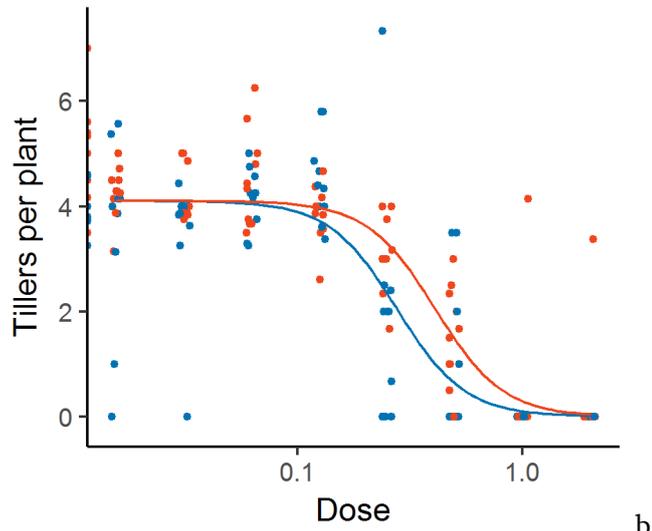
## —The Implications of Spatially Variable Pre-Emergence Herbicide Efficacy for Weed Management

**Table S5.1.** Fitted parameter values for the log-logistic model used to describe the dose-response of the number of tillers per plant of *A. myosuroides* seedlings surviving six weeks after the application of two pre-emergence herbicides on three levels of soil organic matter.

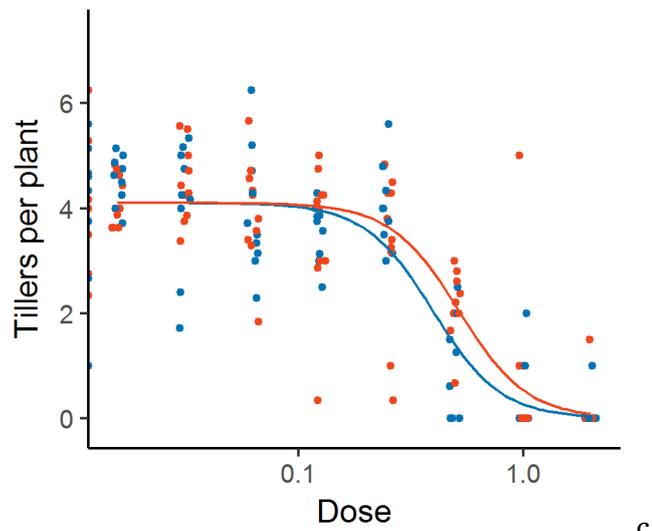
Parameter	Estimate	Standard error
$b$	2.870	0.3570
$d$	4.101	0.0698
$\eta$ – low organic matter, flufenacet	0.086	0.0083
$\eta$ – low organic matter, pendimethalin	0.154	0.0145
$\eta$ – medium organic matter, flufenacet	0.276	0.0264
$\eta$ – medium organic matter, pendimethalin	0.409	0.0423
$\eta$ – high organic matter, flufenacet	0.395	0.0330
$\eta$ – high organic matter, pendimethalin	0.516	0.0083



a



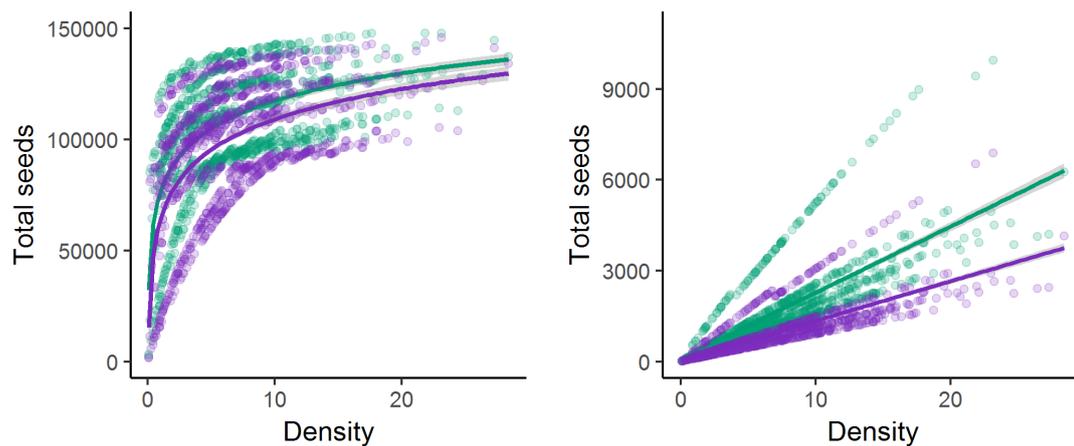
b



c

Figure S5.1. Figure legend on page 237.

**Figure S5.1.** (Figure on page 236.) The number of tillers per plant surviving six weeks after the application of two pre-emergence herbicides on soil with varying levels of organic matter: (a) low, (b) medium and (c) high. Points indicate the response of each sample and the fitted model is shown by a solid line (flufenacet in blue, pendimethalin in red). Dose is given as a proportion of recommended field rate.



**Figure S5.2.** Outputs from 100 simulations for each of 10 years of weather data from the INTERCOM model (a) in the absence of crop competition and (b) in the presence of crop competition. Data points when there is no size penalty to having been sprayed with pre-emergence herbicide are shown in green (mortality adjusted according to inputs in Table 6, no reduction in seedling biomass), those with a size penalty for a sub-lethal dose of herbicide are shown in purple (Mortality and seedling biomass adjusted according to inputs in table 6). A linear model that best describes the data is shown with 95% confidence intervals. (For panel (a) the linear model was fitted to log densities. The back transformed model is shown here).

**Supplementary Material: Chapter 6**  
**— Modelling the Spatial Variation**  
**in *Alopecurus myosuroides* due to**  
**Soil Properties**

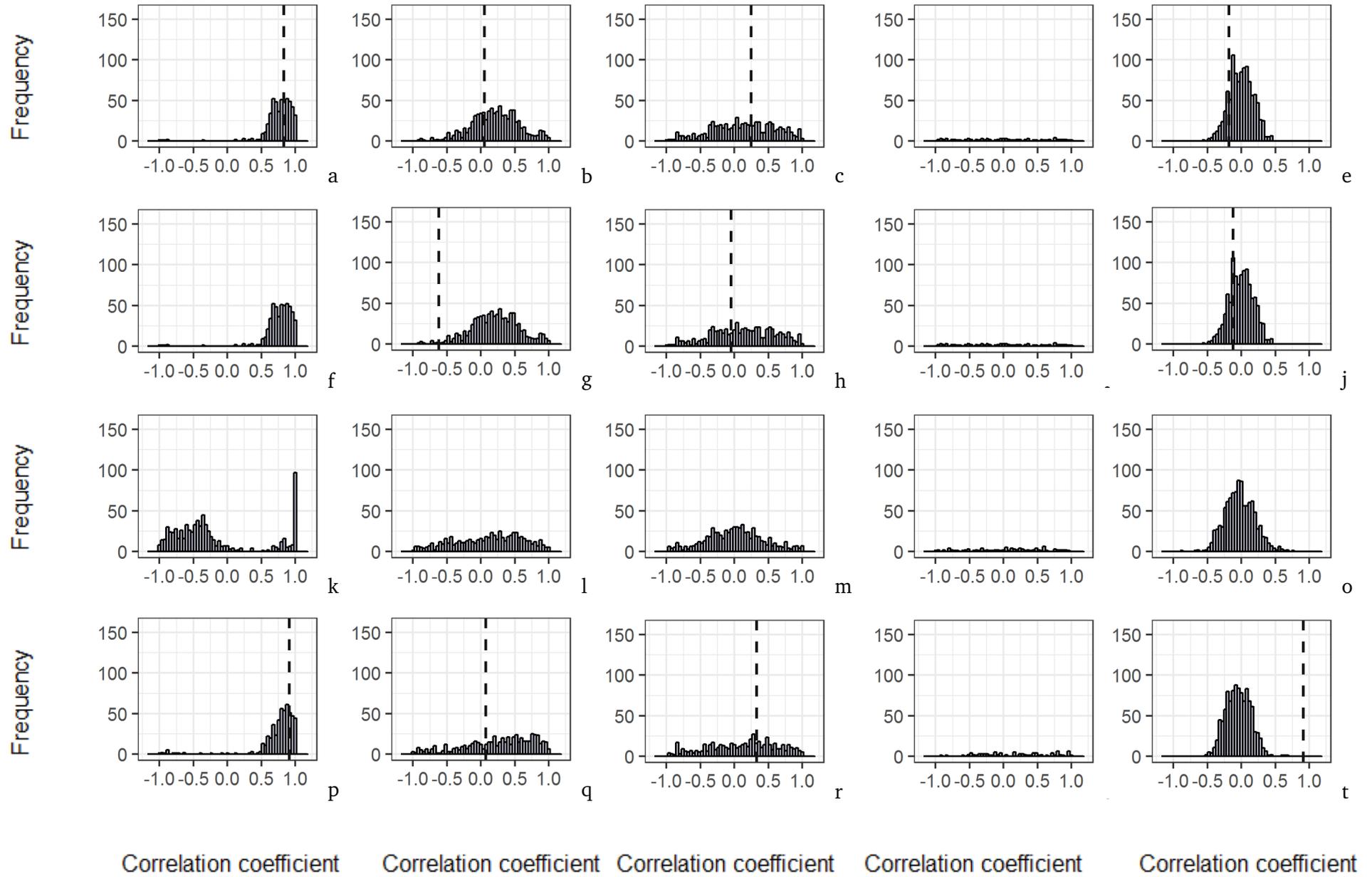


Figure S6.1. Figure legend on page 241

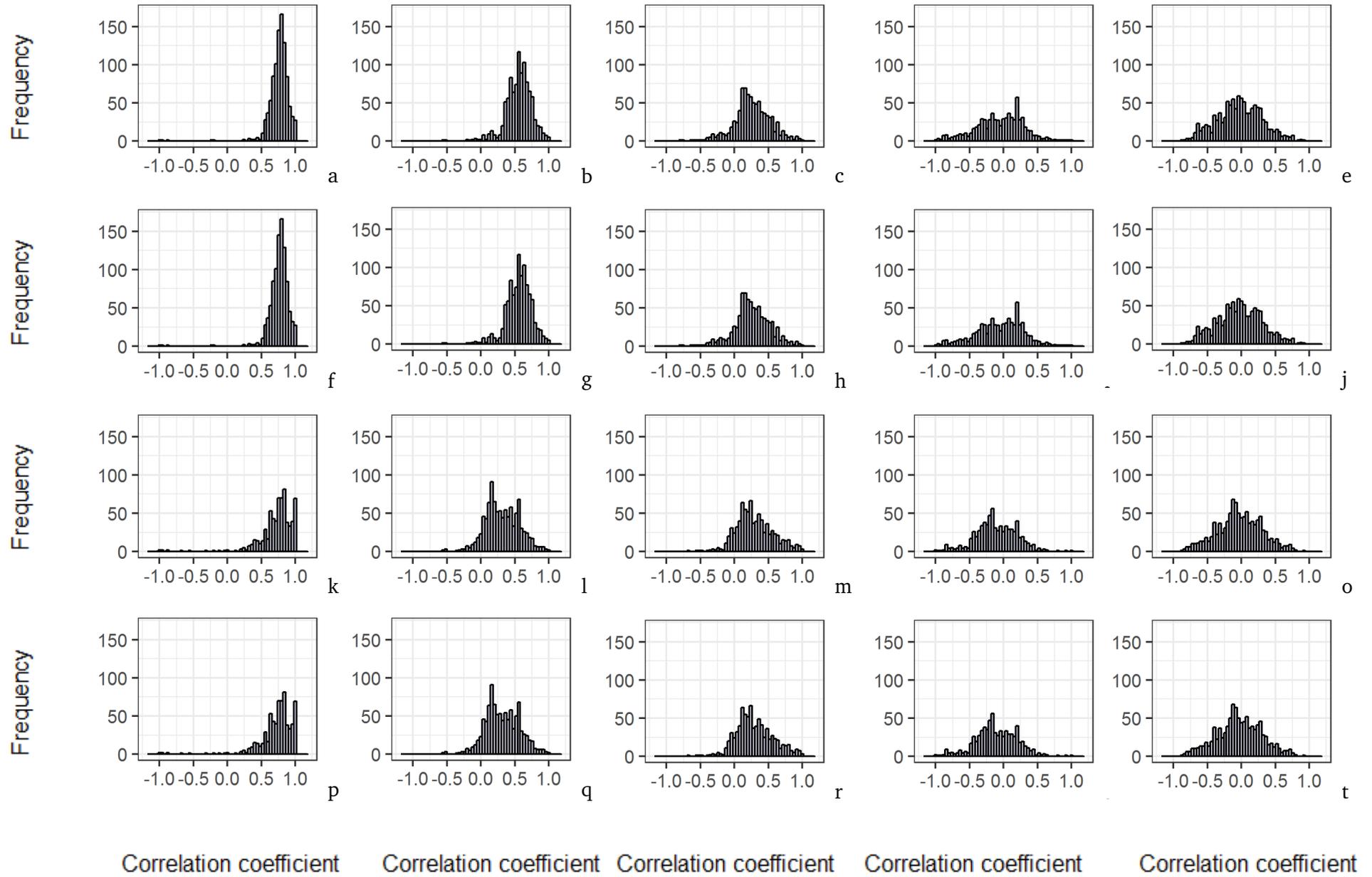


Figure S6.2. Figure legend on page 241

**Figure S6.1.** (Figure on page 239) Frequency distribution of scale-dependent correlation coefficients between the simulated number of *A. myosuroides* heads and simulated soil properties used as inputs into the model model simulations for the field in Harpenden. The corellations shown are between blackgrass heads and the soil properites clay (a–e), soil organic matter (f–j), pH (k–o) and water (p–t) and for each soil property a range of scales are considered ranging from coarse-scale in the first column to fine-scale in teh last column: 50+ m (a, f, k, p), 20 m (b, g, l, q), 7.3 m (c, h, m, r), 2.7 m (d, i, n, s), 1 m (e, j, o, t).

**Figure S6.2.** (Figure on page 240)Frequency distribution of scale-dependent correlation coefficients between the simulated number of *A. myosuroides* heads and simulated soil properties used as inputs into the model model simulations for the field in Haversham. The corellations shown are between blackgrass heads and the soil properites clay (a–e), soil organic matter (f–j), pH (k–o) and water (p–t) and for each soil property a range of scales are considered ranging from coarse-scale in the first column to fine-scale in teh last column: 50+ m (a, f, k, p), 20 m (b, g, l, q), 7.3 m (c, h, m, r), 2.7 m (d, i, n, s), 1 m (e, j, o, t).

The following code is the complete spatial model of the *A. myosuroides* life cycle as described in chapter 6.

The main program file is “Weeds.2.cpp”. This file calls other functions listed in “Grow.cpp” and “Water.cpp”. The “LandGrid.cpp” file contains code to store and access the information about each cell in the grid and “Weather.cpp” contains code to store and access the weather data. These two files (“LandGrid.cpp” and “Weather.cpp”) are taken from an existing crop model whilst the other files comprise my own work.

```
// Weeds_2.cpp : Defines the entry point for the console application.
//

#include <iostream> //indicate all the files to include
#include <direct.h> //header file provided by Microsoft - contains functions for
    manipulating file system directories
#include <fstream> //read/write functions
#include "stdafx.h" //describes both standard system and project specific include
    files
#include "LandGrid.h" //my other files
#include "Grow.h"
#include "Water.h"
#include "Weather.h"
#include <math.h> // a set of functions to compute common mathematical operations
    and transformations
#include <random>
#include "d:\\Program Files (x86)\\NAG\\FL25\\fld11254m1\\c_headers\\nagmk25.h"

int _tmain(int argc, _TCHAR* argv[]) //START HERE
{
    //*****Input files*****//
    char path_buffer[_MAX_PATH]; //declare character
    char Npath_buffer[_MAX_PATH];
    char Cpath_buffer[_MAX_PATH];
    char Opath_buffer[_MAX_PATH];
    char Wpath_buffer[_MAX_PATH];
    char Spath_buffer[_MAX_PATH];
    char Gpath_buffer[_MAX_PATH];
    char Apath_buffer[_MAX_PATH];
    char Ppath_buffer[_MAX_PATH];
    _getcwd(path_buffer, _MAX_PATH); //Gets current working directory
    char drive[_MAX_DRIVE];
    char dir[_MAX_DIR];
    char fname[_MAX_FNAME];
    char ext[_MAX_EXT];
    _splitpath_s(path_buffer, drive, dir, fname, ext); //Splits the working
    directory into drive, directory etc
    strcpy_s(Npath_buffer, drive);
    strcat_s(Npath_buffer, dir);
    int WeathYear(1966);
    strcat_s(Npath_buffer, "Weather\\MetRR."); //Creates the directory path for the
    weather data that we shall read in

    strcpy_s(Cpath_buffer, drive);
    strcat_s(Cpath_buffer, dir);
    strcat_s(Cpath_buffer, "InputData\\scaleHAVclayout1.txt"); //Creates the
    directory path for the clay data that we shall read in
    strcpy_s(Opath_buffer, drive);
    strcat_s(Opath_buffer, dir);
    strcat_s(Opath_buffer, "InputData\\scaleHAVomout1.txt"); //Creates the
    directory path for the OM data that we shall read in
    strcpy_s(Wpath_buffer, drive);
    strcat_s(Wpath_buffer, dir);
    strcat_s(Wpath_buffer, "InputData\\scaleHAVwaterout1.txt"); //Creates the
    directory path for the water data that we shall read in
    strcpy_s(Spath_buffer, drive);
```

```

strcat_s(Spath_buffer, dir);
strcat_s(Spath_buffer, "InputData\\scaleHAVsiltout1.txt"); //Creates the
    directory path for the silt data that we shall read in
strcpy_s(Gpath_buffer, drive);
strcat_s(Gpath_buffer, dir);
strcat_s(Gpath_buffer, "InputData\\HavSlopefull.txt"); //Creates the directory
    path for the slope data that we shall read in
strcpy_s(Apath_buffer, drive);
strcat_s(Apath_buffer, dir);
strcat_s(Apath_buffer, "InputData\\HavAspectfull.txt"); //Creates the directory
    path for the aspect data that we shall read in
strcpy_s(Ppath_buffer, drive);
strcat_s(Ppath_buffer, dir);
strcat_s(Ppath_buffer, "InputData\\scaleHAVphout1.txt"); //Creates the
    directory path for the aspect data that we shall read in

try {

    //*****Set up the field*****//
    Grid::InitialiseGrid(); //Run the initialise grid function - basic function
        to set up a uniform grid with sensible values
    Grid::InitialiseOC(Opath_buffer); // Initialise reading in from OC file
    Grid::InitialiseClay(Cpath_buffer); // Initialise reading in from Clay file
    Grid::InitialiseSWC(Wpath_buffer); // Initialise reading in from Water file
    Grid::InitialiseSilt(Spath_buffer); // Initialise reading in from Silt file
    Grid::InitialiseSlope(Gpath_buffer); // Initialise reading in from Slope
        file
    Grid::InitialiseAspect(Apath_buffer); // Initialise reading in from Aspect
        file
    Grid::InitialisePH(Ppath_buffer); // Initialise reading in from Aspect file

    refsolar(); //Get reference value for solar energy and compute total
        potential energy for each cell in the field. Compare them to the
        reference to give a scaling factor for each cell dependent on slope and
        aspect

    for (int irow = 0; irow < Grid::GetNumRows(); irow++)
    {
        for (int jcol = 0; jcol < Grid::GetNumCols(); jcol++) //For each cell in
            the field
        {
            double myOC = Grid::GetOC(irow, jcol); //get the OM value from the
                grid
            double myClay = Grid::GetClay(irow, jcol); //get the clay value from
                the grid
            double mySilt = Grid::GetSilt(irow, jcol); //get the silt value from
                the grid
            double mybulkd = 0.80806 + (0.823844*exp(-0.27993*myOC) +
                (0.0014065*(1 - myClay - mySilt)) - (0.0010299*myClay)); //
                calculate Db from the soil parameters
            Grid::SetBulkD(irow, jcol, mybulkd); //set Db to the grid
            double myWater = Grid::GetSWC(irow, jcol); //get the water from the
                grid (data input as GWC%)
            myWater = (myWater*mybulkd) / 100; //convert to VWC as a proportion
            Grid::SetSWC(irow, jcol, myWater); //save the VWC proportion to the
                grid
        }
    }
}

```

```

    }
}

int const numyears = 40; //Declare how many years to run the model for

int cult[numyears]; //Define the type of cultivation to be used each year. ↗
    Cultivation type: 0=plough, 1=tine<5, 2=tine 10, 3=tine 20

for (int icount = 0; icount < numyears; icount++)//for each year
{
    cult[icount] = 1; //set cultivation type
    double myadd = floor(fmod(double(icount), 4.0));//every fourth year set ↗
        a different cultivation type
    if (myadd == 1)
    {
        cult[icount] = 0;
    }
}

double breakcrop[numyears]; // Determine whether breakcrops will be used. A ↗
    breakcrop prevents weed from growing in that year but seeds are still ↗
    moved around within the soil due to cultivation. Breakcrop: 0 = no ↗
    breakcrop(normal weed growth), 1 = breakcrop

for (int icount = 0; icount < numyears; icount++)//for each year
{
    breakcrop[icount] = 0;//set there to be no breakcrop
    //double myadd = floor(fmod(double(icount), 8.0));//every eighth year ↗
        set a breakcrop
    //if (myadd == 1)
    //{
    //    breakcrop[icount] = myadd;
    //}

}

//*****Set up dispersal options*****//
//***** Natural dispersal*****//
std::vector<double> proportions;
double extra;

// Natural dispersal is modelled by a rotated Gaussian function as ↗
    described in Paice et al 1998
double mu = 0; // Mean Gaussian seed dispersal distance (0.0m in Paice et ↗
    al, 1988)
double sigma = 0.3;// Standard deviation for Gaussian seed dispersal ↗
    distance (0.3m in Paice et al, 1988)

// By integrating the dispersal functions it is possible to determine the ↗
    proportion of seeds from each grid cell that will be dispersed to other ↗
    grid cells. This function only needs to be run once as the result is a ↗
    proportion which can then be applied year on year to the model no matter ↗
    how many plants there are in each cell. For natural dispersal seeds are ↗
    allocated to cells in turn by integrating different areas under the curve ↗

```

```
    in order according to figure shown in lab book 1 (p15) with seeds first ↗
    falling in the starting square and then the squares immediately adjacent, ↗
    followed by further squares getting ever further from the starting ↗
    point.
natDisp(proportions, extra, mu, sigma); //This function is in Grow.cpp it ↗
    gives 'proportions' and 'extra'. proportions is the proportion of seeds ↗
    that go into each cell type (determined by the distance from the centre ↗
    point). Extra is any remaining proportion after we have integrated up to ↗
    0.999.

//***** Cultivation dispersal*****//
std::vector<double> proportions2;
double extra2;

//Dispersal by cultivation is described in Paice et al (1988) as a Gaussian ↗
    and exponential distribution where the Gaussian distribution(Mean = ↗
    0.025m, stdev = 0.15m) is used for values <= 0 and the exponential ↗
    bistribution(b = 1.68m - 1) is used for values >1. Here, an exponentially ↗
    modified Gaussian distribution is used and the parameters adjusted to ↗
    provide a distribution similar to that provided by Paice et al(1998).
double eta = -0.15; // Mean of the exponentially modified Gaussian ↗
    distribution(-0.15 provides best estimate of data)
double lambda = 0.1; // Std dev of the exponentially modified Gaussian ↗
    distribution(-0.1 provides best estimate of data)
double b = 0.3; // exponential model component of the exponentially ↗
    modified Gaussian distribution(0.3 provides best estimate of data)
int maxdisp = 20; // Set the maximum dispersal distance in m(20m in Paice ↗
    et al, 1998)

cultDisp(proportions2, extra2, lambda, eta, b); //This function is in ↗
    Grow.cpp it gives 'proportions2' and 'extra2'.These describe the ↗
    proportion of seeds that move to each cell along the line of cultivation ↗
    and the extra that is not allocated to any cell by this function

//*****SETUP WATER*****//

double startday = 76; //This is the Julian day for which the soil water ↗
    content is valid - so the day the field measurments were taken
    //CrossF = 21
    //Redb = 71
    //Iv = 85
    //Hav 76

//set flower and harvest day
//This sets up the nag functions to calculate the selection of a random ↗
    number from a normal distrivution
int const LR = 1;
double R[LR];
double X[1];
int ifail = 1;
int const genid(1);
int const subid(0);
int lstate(17);
int* state; //when we declare 'state' we dont say how long it will be so we ↗
```

```

    need to delete it after we have used it
state = new int[lstate]; //here we declare state again so must delete it  ↗
    again
ifail = 1;
G05KGF(genid, subid, state, lstate, ifail); //this is a non-repeatable seed
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05KGF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
int N = 1; // number of numbers to generate

int flowerday = 150; //Julian day for the start of flowering
double var = 3; //variance for distribution for flowering day
G05SKF(N, flowerday, var, state, X, ifail); //take flowering day from a  ↗
    normal distribution
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05SKF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
flowerday = round(X[0]);
int nextharvestday = 206; //Julian day for harvest
var = 6;
G05SKF(N, nextharvestday, var, state, X, ifail); //take harvest day from a  ↗
    normal distribution
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05SKF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
nextharvestday = round(X[0]);
delete[] state; //here we delete 'state'
double mydeficit=0;
Weath::ReadInWeath(0, Npath_buffer, WeathYear); //Read in the first weather  ↗
    file
double myWater;
for (int irow = 0; irow < Grid::GetNumRows(); irow++)
{
    for (int jcol = 0; jcol < Grid::GetNumCols(); jcol++) //for each cell  ↗
        in the field
        {
            myWater = Grid::GetSWC(irow, jcol); //get the water stored in the  ↗
                grid (this is valid for the startday)
            initialwater(irow, jcol, myWater, startday, flowerday); //Take water  ↗
                from start day to flowering
            Grid::SetSWC(irow, jcol, myWater); //set soil water content at the  ↗

```

```

        start of flowering to the grid
        waterdeficit(irow, jcol, myWater, flowerday, nextharvestday,
        mydeficit);//calculate the water deficit from flowering to
        harvest (this is needed in the germination calculations)
        Grid::SetWD(irow, jcol,mydeficit);//set water deficit to the grid
        for season prior to model start
        Grid::SetSWC(irow, jcol, myWater);//set soil water content at
        harvest to the grid
    }
}
////*****Life
cycle*****//
double dropSeeds, aPlants, Heads;

for (int iyear = 0; iyear < numyears; iyear++) //allow the model to run for
the number of years stored in numyears
{
    int thisharvestday = nextharvestday;//we always have the previous year
    and this year in consideration so have to transfer dates in each
    iteration of the model

    //This sets up the nag functions to calculate the selection of a random
    number from a normal distrivution
    int const LR = 1;
    double R[LR];
    double X[1];
    int ifail = 1;
    int const genid(1);
    int const subid(0);
    int lstate(17);
    int* state; //when we declare 'state' we dont say how long it will be
    so we need to delete it after we have used it
    state = new int[lstate]; //here we declare state again so must delete
    it again
    ifail = 1;
    G05KGF(genid, subid, state, lstate, ifail); //this is a non-repeatable
    seed
    int N = 1; // number of numbers to generate
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05KGF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }

    nextharvestday = 220;//Julian day for harvest
    var = 6;//variation in harvest day
    G05SKF(N, nextharvestday, var, state, X, ifail);//take harvest day from
    a normal distribution
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05SKF ";

```

```

        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    nextharvestday = round(X[0]);

    flowerday = 110;//Julian day for the start of flowering //150
    var = 3;//variance for flowering day
    G05SKF(N, flowerday, var, state, X, ifail);//take flowering day from a ↗
    normal distribution
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05SKF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    flowerday = round(X[0]);

    int cultivationday = 258;//Julian day for cultivation
    var = 8;//variance for cultivation day
    G05SKF(N, cultivationday, var, state, X, ifail);//take cultivation day ↗
    from a normal distribution
    if (ifail != 0)
        if (ifail != 0)
        {
            char myText[10];
            _itoa_s(ifail, myText, 10);
            char myBigText[50] = " Error in Nag G05SKF ";
            strcat_s(myBigText, myText);
            throw std::logic_error(myBigText);
        }
    cultivationday = round(X[0]);
    delete[] state; //here we delete 'state'

    if (breakcrop[iyear] == 0) //if there is no breakcrop the weeds will ↗
    grow
    {
        //go through each grid cell in turn and determne how many plants ↗
        grow and what seeds get dropped
        for (int irow = 0; irow < Grid::GetNumRows(); irow++)
        {
            for (int jcol = 0; jcol < Grid::GetNumCols(); jcol++)
            {
                double EarlysumVWC = 0;//we need to calculated the ↗
                accumulated available water throughout the growing season
                int Earlycountdays = 1;
                double LatesumVWC = 0;
                int Latecountdays = 1;
                growearly(irow, jcol, aPlants, thisharvestday, EarlysumVWC, ↗
                Earlycountdays, Heads, cultivationday); //This a function in ↗
                grow.cpp it performs the early part of the life cycle in each ↗
                cell (up to the end of the calendar year)
                Weath::ClearWeath(0);
                Weath::ReadInWeath(0, Npath_buffer, WeathYear + iyear + ↗
                1); //Read in the weather for the next year.
            }
        }
    }

```

```
        growlate(irow, jcol, dropSeeds, aPlants, Earlycountdays,  ↵
        Heads, nextharvestday, flowerday, LatesumVWC,          ↵
        Latecountdays); //This a function in grow.cpp it performs the ↵
        late part of the life cycle in each cell (from the start of ↵
        the calendar year)
    }
}

Disp(proportions); //this does the natural dispersal based on the ↵
proportions calculated for each cell type. It is a function in ↵
grow.cpp. The dispersed seeds are in TempWeeds
}
else //if there is a breakcrop no plants grow and no seeds are dropped
{
    for (int irow = 0; irow < Grid::GetNumRows(); irow++)
    {
        for (int jcol = 0; jcol < Grid::GetNumCols(); jcol++)
        {
            Grid::SetPlants(irow, jcol, 0); //set (to the grid) the ↵
            number of mature plants at the end of the growing season ↵
            Grid::SetDropSeeds(irow, jcol, 0); //set (to the grid) the ↵
            number of dropped seeds
        }
    }
}

// We now have values for the number of plants that grow and where ↵
their seeds have been naturally dispersed to

//*****Movement of seeds in the soil*****//
soilMove(iyear, cult[iyear]); //this converts all seeds in the soil to ↵
old seeds and puts the newly dropped seeds stored in TempWeeds into ↵
the soil surface layer as new seeds, seeds are moved between soil ↵
layers according to the cultivation type. It is a function in ↵
grow.cpp

//Depending on cultivation type seeds in the soil are dispersed in the ↵
direction of cultivation using the proportions found in ↵
proportions2//

if (cult[iyear] == 0) //If the cultivation type is plough, seeds in all ↵
soil layers will be moved in the direction of cultivation
{
    cdisp2NSS(proportions2, extra2, maxdisp); //movement of new seeds ↵
    in the shallow soil layer
    cdisp2NSD(proportions2, extra2, maxdisp); //movement of new seeds ↵
    in the deep soil layer
    cdisp2OSS(proportions2, extra2, maxdisp); //movement of old seeds ↵
    in the shallow soil layer
    cdisp2OSD(proportions2, extra2, maxdisp); //movement of old seeds ↵
    in the deep soil layer
}
else //For other cultivation types, only seeds in the shallow soil ↵
layer will be moved in the direction of cultivation
{
    cdisp2NSS(proportions2, extra2, maxdisp); //movement of new seeds in ↵
```

```
        the shallow soil layer
        cdisp2OSS(proportions2, extra2, maxdisp);//movement of old seeds in
        the shallow soil layer

    } //End of deciding how to disperse seeds in soil according to
    cultivation type

    WriteSeedlings(iyear);//write to a file the number of seedlings that
    emerged this year in each cell
    WriteHeads(iyear);//write to a file the number of heads produced this
    year in each cell
    WriteSWC(iyear);//write out the at the end of this year in each cell
    Writepropavailablewater(iyear);//write out the proportion of available
    water this year in each cell

} //Year Loop

}
catch (std::logic_error &E)
{
    char Mess[500];
    strcpy_s(Mess, E.what());
    std::cout << Mess << '\n';
    system("pause>nul");
}

return 0;
}
```

```
#include "LandGrid.h"
#include <iostream>
#include <fstream>
#include <algorithm>
#include <direct.h>
#include <string>

//The LandGrid allows us to store information about each cell that can be accessed ↗
//in any function

struct TCell { //list of the attributes of a cell

    double Latitude;
    double Elevation;
    double Slope;
    double Aspect;
    double SolarScale;
    double Clay;
    double SoilDepth;
    double Silt;
    double BulkD;
    double pH;
    double OC;
    double SoilWaterContent;
    double WaterDeficit;
    double propavailablewater;
    double EarlySumVWC;

    //Weed properties
    double NewSeeds[2]; //The number of new seeds in the surface soil layer[0], The ↗
        number of new seeds in the deep soil layer[1].
    double OldSeeds[2]; //The number of old seeds in the surface soil layer[0], The ↗
        number of old seeds in the deep soil layer[1].

    double DroppedSeeds; //keeps track of seed that are shed
    double TempSeeds; //keeps track of seed that are shed following dispersal

    double Plants; //The number of mature plants
    double Seedlings; //The number of seedlings in the autumn
    double Heads; //The number of heads produced

};

namespace Grid
{ //set up the size of the field and grid cells - this is different for each field
    // Harpenden
    //int const Nrows=352;
    //int const Ncols=283;
    //Redbourn
    //int const Nrows=421;
    //int const Ncols=371;
    //Ivinghoe
    //int const Nrows=502;
```

```
//int const Ncols=696;
//Haversham
int const Nrows=321;
int const Ncols=272;

double const Cell = 1; // the side length of a grid cell in m
double CultWidth = 40;
double IntVars[2]; //stores values of mu and sigma for natural dispersal
double IntVarsCult[3]; //stores values of mu and sigma for natural dispersal
TCell MainGrid[Nrows][Ncols];

//*****\

void SetIntVars(double mu, double sigma) //A function that allows you to set ↗
    the values of mu and sigma for natural dispersal
{
    IntVars[0] = mu;
    IntVars[1] = sigma;
}

void GetIntVars(double& mu, double& sigma) //A function that allows you to get ↗
    the values of mu and sigma for natural dispersal
{
    mu = IntVars[0];
    sigma = IntVars[1];
}

//*****\

void SetIntVarsCult(double lambda, double eta, double gamma) //A function that ↗
    allows you to set the values of mu and sigma for natural dispersal
{
    IntVarsCult[0] = lambda;
    IntVarsCult[1] = eta;
    IntVarsCult[2] = gamma;
}

void GetIntVarsCult(double& lambda, double& eta, double& gamma) //A function ↗
    that allows you to get the values of mu and sigma for natural dispersal
{
    lambda = IntVarsCult[0];
    eta = IntVarsCult[1];
    gamma = IntVarsCult[2];
}

//*****\

void SetNewSeeds(int irow, int jcol, double myNSeeds[]) //A function that ↗
    allows you to set the values for new seeds in the shallow [0] and deep [1] ↗
    layers
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        for (int ccount = 0; ccount<2; ccount++)
            MainGrid[irow][jcol].NewSeeds[ccount] = myNSeeds[ccount];
    }
}
```

```
    else
    {
        throw std::logic_error("Error in SetNewSeeds: index not in grid");
    }
}

void SetOldSeeds(int irow, int jcol, double myOldSeeds[])//A function that allows you to set the values for old seeds in the shallow [0] and deep [1] layers
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        for (int ccount = 0; ccount<2; ccount++)
            MainGrid[irow][jcol].OldSeeds[ccount] = myOldSeeds[ccount];
    }
    else
    {
        throw std::logic_error("Error in SetOldSeeds: index not in grid");
    }
}

void SetLatitude(int irow, int jcol, double myLat) //A function that allows you to set the latitude - this is needed for meteorological functions
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].Latitude=myLat;
    }
    else
    {
        throw std::logic_error("Error in SetLatitude: index not in grid");
    }
}

void SetElevation(int irow, int jcol, double myEle) //A function that allows you to set the elevation
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].Elevation=myEle;
    }
    else
    {
        throw std::logic_error("Error in SetElevation: index not in grid");
    }
}

void SetPH(int irow, int jcol, double myPH) //A function that allows you to set the pH
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].pH=myPH;
    }
    else
    {
```

```
        throw std::logic_error("Error in SetPH: index not in grid");
    }
}

void SetOC(int irow, int jcol, double myOC) //A function that allows you to set
the organic carbon
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].OC = myOC;
    }
    else
    {
        throw std::logic_error("Error in SetOC: index not in grid");
    }
}

void SetClay(int irow, int jcol, double myClay) //A function that allows you to
set the clay content
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].Clay = myClay;
    }
    else
    {
        throw std::logic_error("Error in SetClay: index not in grid");
    }
}

void SetSilt(int irow, int jcol, double mySilt) //A function that allows you to
set the silt content
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].Silt = mySilt;
    }
    else
    {
        throw std::logic_error("Error in SetSilt: index not in grid");
    }
}

void SetBulkD(int irow, int jcol, double myBulkD) //A function that allows you
to set the bulk density
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].BulkD = myBulkD;
    }
    else
    {
        throw std::logic_error("Error in SetBulkD: index not in grid");
    }
}
```

```
void SetSWC(int irow, int jcol, double mySWC) //A function that allows you to ↗
set the soil water content
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].SoilWaterContent=mySWC;
    }
    else
    {
        throw std::logic_error("Error in SetSWC: index not in grid");
    }
}

void Setpropavailablewater(int irow, int jcol, double propavailablewater) //A ↗
function that allows you to set the proportion of available soil water
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].propavailablewater = propavailablewater;
    }
    else
    {
        throw std::logic_error("Error in Setpropavailablewater: index not in ↗
grid");
    }
}

void SetEarlySumVWC(int irow, int jcol, double EarlySumVWC) //A function that ↗
allows you to set the sum of available water in the early part of the year
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].EarlySumVWC = EarlySumVWC;
    }
    else
    {
        throw std::logic_error("Error in SetEarlySumVWC: index not in grid");
    }
}

void SetWD(int irow, int jcol, double myeWD) //A function that allows you to ↗
set the soil water deficit
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].WaterDeficit = myeWD;
    }
    else
    {
        throw std::logic_error("Error in SetWD: index not in grid");
    }
}
```

```
void SetSoilDepth(int irow, int jcol, double mySoilDepth) //A function that ↗
allows you to set the soil depth
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].SoilDepth = mySoilDepth;
    }
    else
    {
        throw std::logic_error("Error in SetSoilDepth: index not in grid");
    }
}

void SetSlope(int irow, int jcol, double mySlope) //A function that allows you ↗
to set the slope
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].Slope=mySlope;
    }
    else
    {
        throw std::logic_error("Error in SetSlope: index not in grid");
    }
}

void SetAspect(int irow, int jcol, double myAspect) //A function that allows ↗
you to set the aspect
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].Aspect = myAspect;
    }
    else
    {
        throw std::logic_error("Error in SetAspect: index not in grid");
    }
}

void SetSolarScale(int irow, int jcol, double mySolarScale) //A function that ↗
allows you to set the solar scalar
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        MainGrid[irow][jcol].SolarScale = mySolarScale;
    }
    else
    {
        throw std::logic_error("Error in SetSolarScale: index not in grid");
    }
}

//*****\
```

```
void GetNewSeeds(int irow, int jcol, double myNSeeds[]) //A function that ↗
allows you to get the values for new seeds in the shallow [0] and deep [1] ↗
layers
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        for (int ccount = 0; ccount<2; ccount++)
            myNSeeds[ccount] = MainGrid[irow][jcol].NewSeeds[ccount];
    }
    else
    {
        throw std::logic_error("Error in GetNewSeeds: index not in grid");
    }
}

void GetOldSeeds(int irow, int jcol, double myOSeeds[]) //A function that ↗
allows you to get the values for old seeds in the shallow [0] and deep [1] ↗
layers
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        for (int ccount = 0; ccount<2; ccount++)
            myOSeeds[ccount] = MainGrid[irow][jcol].OldSeeds[ccount];
    }
    else
    {
        throw std::logic_error("Error in GetOldwSeeds: index not in grid");
    }
}

double GetLatitude(int irow, int jcol) //A function that allows you to get the ↗
latitude - this is needed for meteorological functions
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].Latitude;
    }
    else
    {
        throw std::logic_error("Error in GetLat: index not in grid");
    }
}

double GetElevation(int irow, int jcol) //A function that allows you to get the ↗
elevation
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].Elevation;
    }
    else
    {
        throw std::logic_error("Error in GetElevation: index not in grid");
    }
}
```

```
}

double GetClay(int irow, int jcol) //A function that allows you to get the clay ↗
content
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].Clay;
    }
    else
    {
        throw std::logic_error("Error in GetClay: index not in grid");
    }
}

double GetSilt(int irow, int jcol)//A function that allows you to get the silt ↗
content
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].Silt;
    }
    else
    {
        throw std::logic_error("Error in GetSilt: index not in grid");
    }
}

double GetBulkD(int irow, int jcol) //A function that allows you to get the ↗
bulk density
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].BulkD;
    }
    else
    {
        throw std::logic_error("Error in GetSilt: index not in grid");
    }
}

double GetSWC(int irow, int jcol) //A function that allows you to get the soil ↗
water content
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].SoilWaterContent;
    }
    else
    {
        throw std::logic_error("Error in SetSWC: index not in grid");
    }
}

double Getpropavailablewater(int irow, int jcol) //A function that allows you ↗
```

```
    to get the soil water content
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].propavailablewater;
    }
    else
    {
        throw std::logic_error("Error in Getpropavailablewater: index not in grid");
    }
}

double GetEarlySumVWC(int irow, int jcol) //A function that allows you to get
the soil water content
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].EarlySumVWC;
    }
    else
    {
        throw std::logic_error("Error in GetEarlySumVWC: index not in grid");
    }
}

double GetWD(int irow, int jcol) //A function that allows you to get the soil
water content
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].WaterDeficit;
    }
    else
    {
        throw std::logic_error("Error in GetWD: index not in grid");
    }
}

double GetPH(int irow, int jcol) //A function that allows you to get the pH
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].pH;
    }
    else
    {
        throw std::logic_error("Error in GetPH: index not in grid");
    }
}

double GetOC(int irow, int jcol) //A function that allows you to get the
```

```
    organic carbon
    {
        if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
        {
            return MainGrid[irow][jcol].OC;
        }
        else
        {
            throw std::logic_error("Error in GetOC: index not in grid");
        }
    }

int GetNumRows() //A function that allows you to get the number of rows
{
    return Nrows;
}

int GetNumCols() //A function that allows you to get the number of columns
{
    return Ncols;
}

double GetCell() //A function that allows you to get the cell size
{
    return Cell;
}

double GetCultWidth() //A function that allows you to get the cultivator width
{
    return CultWidth;
}

double GetSoilDepth(int irow, int jcol) //A function that allows you to get the
soil depth
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].SoilDepth;
    }
    else
    {
        throw std::logic_error("Error in GetSoilDepth: index not in grid");
    }
}

double GetSlope(int irow, int jcol) //A function that allows you to get the
soil depth
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].Slope;
    }
    else
    {
        throw std::logic_error("Error in GetSlope: index not in grid");
    }
}
```

```
}

double GetAspect(int irow, int jcol) //A function that allows you to get the soil depth ↗
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].Aspect;
    }
    else
    {
        throw std::logic_error("Error in GetAspect: index not in grid");
    }
}

double GetSolarScale(int irow, int jcol) //A function that allows you to get the soil depth ↗
{
    if ((irow<Nrows)&(irow>-1)&(jcol<Ncols)&(jcol>-1))
    {
        return MainGrid[irow][jcol].SolarScale;
    }
    else
    {
        throw std::logic_error("Error in GetSolarScale: index not in grid");
    }
}

//*****\

void ClearTempWeeds() //A function to clear the vlaues from TempWeeds
{
    for (int icount = 0; icount<Nrows; icount++)
    {
        for (int jcount = 0; jcount<Ncols; jcount++)
        {
            MainGrid[icount][jcount].TempSeeds=0;
        }
    }
}

void SetTempWeed(int irow, int jcol, double NewNum) //A function to set the vlaues from TempWeeds ↗
{
    if ((irow>-1) && (irow<Grid::GetNumRows()) && (jcol>-1) && (jcol < Grid::GetNumCols())) ↗
    {
        MainGrid[irow][jcol].TempSeeds = NewNum;
    }
    else
    {
        throw std::logic_error("index out of bounds");
    }
}
```

```
}

double GetTempWeed(int irow, int jcol) //A function to get the vlaues from TempWeeds
{
    if ((irow>-1) && (irow<Grid::GetNumRows()) && (jcol>-1) && (jcol<Grid::GetNumCols()))
        return MainGrid[irow][jcol].TempSeeds;
    else
        throw std::logic_error("index out of bounds");
}

void SetDropSeeds(int irow, int jcol, double dropSeeds) //A function to set the vlaues in DropSeeds
{
    if ((irow>-1) && (irow<Grid::GetNumRows()) && (jcol>-1) && (jcol<Grid::GetNumCols()))
        MainGrid[irow][jcol].DroppedSeeds = dropSeeds;
    else
        throw std::logic_error("index out of bounds");
}

double GetDropSeeds(int irow, int jcol) //A function to get the vlaues in DropSeeds
{
    if ((irow>-1) && (irow<Grid::GetNumRows()) && (jcol>-1) && (jcol<Grid::GetNumCols()))
        return MainGrid[irow][jcol].DroppedSeeds;
    else
        throw std::logic_error("index out of bounds");
}

void SetPlants(int irow, int jcol, double Plants) //A function to set the vlaues in Plants
{
    if ((irow>-1) && (irow<Grid::GetNumRows()) && (jcol>-1) && (jcol<Grid::GetNumCols()))
        MainGrid[irow][jcol].Plants = Plants;
    else
        throw std::logic_error("index out of bounds");
}

double GetPlants(int irow, int jcol) //A function to get the vlaues in Plants
{
    if ((irow>-1) && (irow<Grid::GetNumRows()) && (jcol>-1) && (jcol<Grid::GetNumCols()))
        return MainGrid[irow][jcol].Plants;
    else
        throw std::logic_error("index out of bounds");
}

void SetSeedlings(int irow, int jcol, double Seedlings) //A function to set the vlaues in Plants
{
    if ((irow>-1) && (irow<Grid::GetNumRows()) && (jcol>-1) &&
```

```

        (jcol<Grid::GetNumCols()))
        MainGrid[irow][jcol].Seedlings = Seedlings;
    else
        throw std::logic_error("index out of bounds");
}

double GetSeedlings(int irow, int jcol) //A function to get the vlaues in Plants
{
    if ((irow > -1) && (irow<Grid::GetNumRows()) && (jcol>-1) && (jcol <
        Grid::GetNumCols()))
        return MainGrid[irow][jcol].Seedlings;
    else
        throw std::logic_error("index out of bounds");
}

void SetHeads(int irow, int jcol, double Heads) //A function to set the vlaues
in Plants
{
    if ((irow>-1) && (irow<Grid::GetNumRows()) && (jcol>-1) &&
        (jcol<Grid::GetNumCols()))
        MainGrid[irow][jcol].Heads = Heads;
    else
        throw std::logic_error("index out of bounds");
}

double GetHeads(int irow, int jcol) //A function to get the vlaues in Plants
{
    if ((irow > -1) && (irow<Grid::GetNumRows()) && (jcol>-1) && (jcol <
        Grid::GetNumCols()))
        return MainGrid[irow][jcol].Heads;
    else
        throw std::logic_error("index out of bounds");
}

//*****\

//Use this for now - a basic set up for a uniform grid
void InitialiseGrid() //A function with a basic set up for the grid
{
    char path_buffer[_MAX_PATH];
    char Npath_buffer[_MAX_PATH];
    _getcwd(path_buffer, _MAX_PATH);
    strcpy_s(Npath_buffer, path_buffer);
    strcat_s(Npath_buffer, "\\OutFiles");
    int dirMade = _mkdir(Npath_buffer);

    for (int icount=0; icount<Grid::GetNumRows(); icount++)
    {
        for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
        {
            //Set the seeds
            double mySeeds[2] = {2000, 8000};
            int mycol = Grid::GetNumCols() / 2; //define the centre square
            int myrow = Grid::GetNumRows() / 2;

```

```
if (icount > myrow - 5 && icount < myrow + 5 && jcount > mycol - 5 &&
    jcount < mycol + 5)
{
    mySeeds[0] = 2000;
    mySeeds[1] = 8000;
}

SetNewSeeds(icount, jcount, mySeeds); //set the new seeds as
described above
SetOldSeeds(icount, jcount, mySeeds); //and the old seeds

SetLatitude(icount, jcount, 51.77); //51.77set latitude to a single
value everywhere
SetElevation(icount, jcount, 100); //set elevation to a single
value everywhere

//SetWeathSet(icount, jcount, 0);

//soil - define some standard values to be used for the whole field

double mypH = 6;
double myClay;
myClay = 23.4;

double mySilt;
mySilt = 36.6;

double myOC;
myOC = 4.7;

double mySWC;
mySWC = 25;

double myDepth = 100; //in mm

double myslope, myaspect;
if (icount==0 && jcount==0)
{
    myslope = 0;
    myaspect = 0;
}
if (icount == 0 && jcount == 1)
{
    myslope = 30;
    myaspect = 45;
}
if (icount == 1 && jcount == 0)
{
    myslope = 30;
    myaspect = 180;
}
if (icount == 1 && jcount == 1)
{
    myslope = 10;
    myaspect = 275;
```

```
    }
    //set these soil parameters for the whole grid
    SetPH(icontains, jcount, mypH);
    SetClay(icontains, jcount, myClay);
    SetSilt(icontains, jcount, mySilt);
    SetSWC(icontains, jcount, mySWC);
    SetOC(icontains, jcount, myOC);
    SetSlope(icontains, jcount, myslope); //set slope to a single value ↗
    everywhere
    SetAspect(icontains, jcount, myaspect); //set slope to a single value ↗
    everywhere
    SetSoilDepth(icontains, jcount, myDepth); //set the soil depth - LOOK ↗
    INTO THIS MORE
}
}
}

//These functions can be worked on to read data files to set up variable soil ↗
across the grid
void InitialisePH(char MyPHData[])
{
    std::ifstream MyFile(MyPHData);
    if (MyFile)
    {
        for (int icount=0; icount<Grid::GetNumRows(); icount++)
        {
            for (int jcount=0; jcount<Grid::GetNumCols(); jcount++)
            {
                if (!MyFile.eof())
                {
                    double MyPH(0);
                    MyFile>>MyPH;
                    SetPH(icontains, jcount, MyPH); //function to set PH
                }
                else
                {
                    throw std::logic_error("PH Input file too short");
                }
            }
        }
    }
    else
    {
        throw std::logic_error("Error opening PH file");
    }
}

void InitialiseSoilDepth(char MySoilDepth[])
{
    std::ifstream MyFile(MySoilDepth);
    if (MyFile)
    {
```

```
int FGridRows, FGridCols; // first check that number of Rows and Cols
    match our grid
char tempData[200];
MyFile.getline(tempData, 200);

MyFile>>FGridRows;
MyFile>>FGridCols;
if ((FGridRows==Grid::GetNumRows())&&(FGridCols==Grid::GetNumCols()))
{
    double* Mshall = new double[FGridRows*FGridCols];

    int kcount=0;
    for (int icount=0; icount<Grid::GetNumRows(); icount++)
    {
        for (int jcount=0; jcount<Grid::GetNumCols(); jcount++)
        {
            if (!MyFile.eof())
            {
                MyFile>>Mshall[kcount];
                kcount++;
            }
            else
            {
                MyFile.close();
                delete [] Mshall;

                Mshall=NULL;

                throw std::logic_error("Sow Input file too short");
            }
        }
    }
    MyFile.getline(tempData, 200);
    MyFile.getline(tempData, 200);

    MyFile.getline(tempData, 200);
    kcount=0;
    for (int icount=0; icount<Grid::GetNumRows(); icount++)
    {
        for (int jcount=0; jcount<Grid::GetNumCols(); jcount++)
        {
            double myDepth=Mshall[kcount];
            SetSoilDepth(icount, jcount, myDepth);
            kcount++;
        }
    }
    delete [] Mshall;
    Mshall=NULL;
}
else
{
    MyFile.close();
    throw std::logic_error("Number of rows and columns in file
        incorrect");
}
```

```
    }
    else
        throw std::logic_error("Error opening SoilDepth file");
}
void InitialiseClay(char MyClay[])
{
    std::ifstream MyFile(MyClay);
    if (MyFile)
    {
        int FGridRows, FGridCols; // first check that number of Rows and Cols match
        our grid
        char tempData[200];
        MyFile.getline(tempData, 200);

        MyFile>>FGridRows;
        MyFile>>FGridCols;
        if ((FGridRows==Grid::GetNumRows())&&(FGridCols==Grid::GetNumCols()))
        {
            double* Mshall = new double[FGridRows*FGridCols];

            int kcount=0;
            for (int icount=0; icount<Grid::GetNumRows(); icount++)
            {
                for (int jcount=0; jcount<Grid::GetNumCols(); jcount++)
                {
                    if (!MyFile.eof())
                    {
                        MyFile>>Mshall[kcount];
                        kcount++;
                    }
                    else
                    {
                        MyFile.close();
                        delete [] Mshall;
                        Mshall=NULL;

                        throw std::logic_error("Sow Input file too short");
                    }
                }
            }
            MyFile.getline(tempData, 200);
            MyFile.getline(tempData, 200);
            kcount=0;

            kcount=0;
            for (int icount=0; icount<Grid::GetNumRows(); icount++)
            {
                for (int jcount=0; jcount<Grid::GetNumCols(); jcount++)
                {
                    double myDepth;
                    myDepth=Mshall[kcount];
                    SetClay(icontains, jcount, myDepth);
                    kcount++;
                }
            }
        }
    }
}
```

```
        }
    }
    delete [] Mshall;

    Mshall=NULL;

}
else
{
    MyFile.close();
    throw std::logic_error("Number of rows and columns in file
        incorrect");
}

}
else
    throw std::logic_error("Error opening Clay file");
}

void InitialiseSWC(char MySWC[])
{
    std::ifstream MyFile(MySWC);
    if (MyFile)
    {
        int FGridRows, FGridCols; // first check that number of Rows and Cols
            match our grid
        char tempData[200];
        MyFile.getline(tempData, 200);

        MyFile >> FGridRows;
        MyFile >> FGridCols;
        if ((FGridRows == Grid::GetNumRows()) && (FGridCols == Grid::GetNumCols()
            ()))
        {
            double* Mshall = new double[FGridRows*FGridCols];

            int kcount = 0;
            for (int icount = 0; icount<Grid::GetNumRows(); icount++)
            {
                for (int jcount = 0; jcount<Grid::GetNumCols(); jcount++)
                {
                    if (!MyFile.eof())
                    {
                        MyFile >> Mshall[kcount];
                        kcount++;
                    }
                    else
                    {
                        MyFile.close();
                        delete[] Mshall;
                        Mshall = NULL;

                        throw std::logic_error("Sow Input file too short");
                    }
                }
            }
        }
    }
}
```

```

    }
    MyFile.getline(tempData, 200);
    MyFile.getline(tempData, 200);
    kcount = 0;

    kcount = 0;
    for (int icount = 0; icount<Grid::GetNumRows(); icount++)
    {
        for (int jcount = 0; jcount<Grid::GetNumCols(); jcount++)
        {
            double myDepth;
            myDepth = Mshall[kcount];
            SetSWC(icount, jcount, myDepth);
            kcount++;
        }
    }
    delete[] Mshall;

    Mshall = NULL;

}
else
{
    MyFile.close();
    throw std::logic_error("Number of rows and columns in file
        incorrect");
}

}
else
    throw std::logic_error("Error opening SWC file");
}
void InitialiseSilt(char MySilt[])
{
    {

        std::ifstream MyFile(MySilt);
        if (MyFile)
        {
            int FGridRows, FGridCols; // first check that number of Rows and
                Cols match our grid
            char tempData[200];
            MyFile.getline(tempData, 200);

            MyFile >> FGridRows;
            MyFile >> FGridCols;
            if ((FGridRows == Grid::GetNumRows()) && (FGridCols ==
                Grid::GetNumCols()))
            {
                double* Mshall = new double[FGridRows*FGridCols];

                int kcount = 0;
                for (int icount = 0; icount<Grid::GetNumRows(); icount++)
                {
                    for (int jcount = 0; jcount<Grid::GetNumCols(); jcount++)

```

```
{
    if (!MyFile.eof())
    {
        MyFile >> Mshall[kcount];
        kcount++;
    }
    else
    {
        MyFile.close();
        delete[] Mshall;
        Mshall = NULL;

        throw std::logic_error("Sow Input file too short");
    }
}
MyFile.getline(tempData, 200);
MyFile.getline(tempData, 200);
kcount = 0;

kcount = 0;
for (int icount = 0; icount < Grid::GetNumRows(); icount++)
{
    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {
        double myDepth;
        myDepth = Mshall[kcount];
        SetSilt(icontains, jcount, myDepth);
        kcount++;
    }
}
delete[] Mshall;

Mshall = NULL;

}
else
{
    MyFile.close();
    throw std::logic_error("Number of rows and columns in file
        incorrect");
}
}
else
    throw std::logic_error("Error opening Silt file");
}
}

void InitialiseBulkD(char MyBulkD[])
{
}

void InitialiseOC(char MyOCData[])
{
    {
```

```
std::ifstream MyFile(MyOCData);
if (MyFile)
{
    int FGridRows, FGridCols; // first check that number of Rows and
    Cols match our grid
    char tempData[200];
    MyFile.getline(tempData, 200);

    MyFile >> FGridRows;
    MyFile >> FGridCols;
    if ((FGridRows == Grid::GetNumRows()) && (FGridCols ==
    Grid::GetNumCols()))
    {
        double* Mshall = new double[FGridRows*FGridCols];

        int kcount = 0;
        for (int icount = 0; icount<Grid::GetNumRows(); icount++)
        {
            for (int jcount = 0; jcount<Grid::GetNumCols(); jcount++)
            {
                if (!MyFile.eof())
                {
                    MyFile >> Mshall[kcount];
                    kcount++;
                }
                else
                {
                    MyFile.close();
                    delete[] Mshall;
                    Mshall = NULL;

                    throw std::logic_error("OM Input file too short");
                }
            }
        }
        MyFile.getline(tempData, 200);
        MyFile.getline(tempData, 200);
        kcount = 0;

        kcount = 0;
        for (int icount = 0; icount<Grid::GetNumRows(); icount++)
        {
            for (int jcount = 0; jcount<Grid::GetNumCols(); jcount++)
            {
                double myDepth;
                myDepth = Mshall[kcount];
                SetOC(icount, jcount, myDepth);
                kcount++;
            }
        }
        delete[] Mshall;

        Mshall = NULL;
    }
}
```

```

        else
        {
            MyFile.close();
            throw std::logic_error("Number of rows and columns in file
            incorrect");
        }

    }
    else
        throw std::logic_error("Error opening OC file");
}

void InitialiseEle(char MyEle[])
{
    std::ifstream MyFile(MyEle);
    if (MyFile)
    {
        int FGridRows, FGridCols; // first check that number of Rows and Cols
        match our grid
        char tempData[200];
        MyFile.getline(tempData, 200);

        MyFile>>FGridRows;
        MyFile>>FGridCols;
        if ((FGridRows==Grid::GetNumRows())&&(FGridCols==Grid::GetNumCols()))
        {
            for (int icount=0; icount<Grid::GetNumRows(); icount++)
            {
                for (int jcount=0; jcount<Grid::GetNumCols(); jcount++)
                {
                    if (!MyFile.eof())
                    {
                        double MyEled(0);
                        MyFile>>MyEled;
                        SetElevation(icontains, jcount, MyEled); //function to set
                        elevation
                    }
                    else
                    {
                        throw std::logic_error("Elevation Input file too
                        short");
                    }
                }
            }
        }
        else
        {
            MyFile.close();
            throw std::logic_error("Number of rows and columns in file
            incorrect");
        }
    }
    else
    {
        throw std::logic_error("Error opening elevation file");
    }
}

```

```
    }  
  
    }  
  
    void InitialiseSlope(char MySlope[])  
    {  
        {  
  
            std::ifstream MyFile(MySlope);  
            if (MyFile)  
            {  
                int FGridRows, FGridCols; // first check that number of Rows and  
                Cols match our grid  
                char tempData[200];  
                MyFile.getline(tempData, 200);  
  
                MyFile >> FGridRows;  
                MyFile >> FGridCols;  
                if ((FGridRows == Grid::GetNumRows()) && (FGridCols ==  
                    Grid::GetNumCols()))  
                {  
                    double* Mshall = new double[FGridRows*FGridCols];  
  
                    int kcount = 0;  
                    for (int icount = 0; icount<Grid::GetNumRows(); icount++)  
                    {  
                        for (int jcount = 0; jcount<Grid::GetNumCols(); jcount++)  
                        {  
                            if (!MyFile.eof())  
                            {  
                                MyFile >> Mshall[kcount];  
                                kcount++;  
                            }  
                            else  
                            {  
                                MyFile.close();  
                                delete[] Mshall;  
                                Mshall = NULL;  
  
                                throw std::logic_error("Slope Input file too  
short");  
                            }  
                        }  
                    }  
                    MyFile.getline(tempData, 200);  
                    MyFile.getline(tempData, 200);  
                    kcount = 0;  
  
                    kcount = 0;  
                    for (int icount = 0; icount<Grid::GetNumRows(); icount++)  
                    {  
                        for (int jcount = 0; jcount<Grid::GetNumCols(); jcount++)  
                        {  
                            double mySlope;  
                            mySlope = Mshall[kcount];
```

```
        SetSlope(icount, jcount, mySlope);
        kcount++;
    }
}
delete[] Mshall;

Mshall = NULL;

}
else
{
    MyFile.close();
    throw std::logic_error("Number of rows and columns in file
incorrect");
}

}
else
    throw std::logic_error("Error opening Slope file");
}
}

void InitialiseAspect(char MyAspect[])
{
    {

        std::ifstream MyFile(MyAspect);
        if (MyFile)
        {
            int FGridRows, FGridCols; // first check that number of Rows and
            Cols match our grid
            char tempData[200];
            MyFile.getline(tempData, 200);

            MyFile >> FGridRows;
            MyFile >> FGridCols;
            if ((FGridRows == Grid::GetNumRows()) && (FGridCols ==
            Grid::GetNumCols()))
            {
                double* Mshall = new double[FGridRows*FGridCols];

                int kcount = 0;
                for (int icount = 0; icount<Grid::GetNumRows(); icount++)
                {
                    for (int jcount = 0; jcount<Grid::GetNumCols(); jcount++)
                    {
                        if (!MyFile.eof())
                        {
                            MyFile >> Mshall[kcount];
                            kcount++;
                        }
                        else
                        {
                            MyFile.close();
                            delete[] Mshall;
                        }
                    }
                }
            }
        }
    }
}
```

```
Mshall = NULL;

        throw std::logic_error("Aspect Input file too
short");
    }
}
MyFile.getline(tempData, 200);
MyFile.getline(tempData, 200);
kcount = 0;

kcount = 0;
for (int icount = 0; icount < Grid::GetNumRows(); icount++)
{
    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {
        double myAspect;
        myAspect = Mshall[kcount];
        SetAspect(icount, jcount, myAspect);
        kcount++;
    }
}
delete[] Mshall;

Mshall = NULL;

}
else
{
    MyFile.close();
    throw std::logic_error("Number of rows and columns in file
incorrect");
}
}
else
    throw std::logic_error("Error opening Aspect file");
}
} // End of namespace
```

```
#include "Grow.h"
#include "math.h"
#include "LandGrid.h"
#include "Water.h"
#include <fstream>
#include <iostream>
#include <direct.h>
#include <vector>
#include <random>

#include "d:\\Program Files (x86)\\NAG\\FL25\\fld11254m1\\c_headers\\nagmk25.h"

void growearly(int irow, int jcol, double& aPlants, int harvestday, double&
    EarlysumVWC, int& Earlycountdays, double& Heads, int cultivationday)
// grow early is a function describing the life cycle of the blackgrass plant from
// germination to the end of the calendar year.
// Inputs are the field size, the dates for harvest and cultivation.
// Outputs are the number of plants in each cell and the amount of water
// accumulated over this period
{
    //water saved in the grid is for harvestday
    double myWater = Grid::GetSWC(irow, jcol);//get the value of water saved in the
    grid
    initialwater(irow, jcol, myWater, harvestday, cultivationday);//move water
    froward from harvest day to cultivation day
    Grid::SetSWC(irow, jcol, myWater);//set SWC in the grid for start of
    cultivation

    double aold = 818; //age of oldseeds
    double MgOld = hydrothermaltime(irow, jcol, aold,cultivationday); //Mean
    germination of old seeds determined by a function hydrothermal time in
    Water.cpp
    double anew = 60; //age of newseeds
    double MgNew = hydrothermaltime(irow, jcol, anew, cultivationday); //Mean
    germination of new seeds determined by a function hydrothermal time in
    Water.cpp

    //// Germination
    // The proportion of seeds which germinate in each square is determined by
    randomly selecting numbers from the distributions defined above for old and
    new seeds in the surface layer of the soil.

    // GermO is the proportion of old seeds germinating in each cell of the field
    double GermO = MgOld;
    GermO = fmax(0, GermO); // The proportion is limited to values between 0 and 1
    GermO = fmin(1, GermO);

    // GermN is the proportion of old seeds germinating in each cell of the field
    double GermN = MgNew;
    GermN = fmax(0, GermN); // The proportion is limited to values between 0 and 1
    GermN = fmin(1, GermN);

    // The number of plants that germinate is calculated by multiplying the seeds
    in the soil by the germination rates
```

```
double myNewS[2], myOldS[2];
Grid::GetNewSeeds(irow, jcol, myNewS);
Grid::GetOldSeeds(irow, jcol, myOldS);

aPlants = (GermO*myOldS[0] + GermN*myNewS[0]);
Grid::SetSeedlings(irow, jcol, aPlants); //The number of seedlings that germinate
    is saved to the grid - This can be compared to autumn seedling counts in the
    field

///// Herbicide Kill
//pre-em
// Herbicide kill acts on a binomial distribution with a probability of
    survival being determined by organic matter. Results from Metcalfe et al 2017
    (dose response paper), with a curve fitted.
double x1 = 4.9; //parameters of the curve
double x2 = 3.8252;
double x3 = -1.0890;
double myOm = Grid::GetOC(irow, jcol); //get the organic matter in each cell.
    This is used in the calculation of herbicide efficacy
double bino = x1*myOm / (1 + x2*myOm) + x3; //bino is the proportion of
    seedlings surviving pre-emergence herbicide

std::default_random_engine generator; //set up a binomial distribution generator
std::binomial_distribution<int> distribution(aPlants, bino);

aPlants = distribution(generator); // Calculate the number of plants remaining
    after pre-em herbicide application.

double postem = 0.3; //survival from post em (independent of soil propoerties)
    - given on Bayer website
std::default_random_engine generator2; //set up binomial distributon
std::binomial_distribution<int> distribution2(aPlants, postem);
aPlants = distribution2(generator2); // Calculate the number of plants
    remaining after post-em herbicide application.

///// Seed Production
// The numebr of heads per plant is density dependent, the numebr of seeds per
    head is calculated from a lognormal distribution and the number of seeds taht
    are viable is stochastically generated from a normal distribution. Seed
    losses are also accounted for using a lognormal distribution
// Moss (1990) describes a density dependent relationship between the number of
    plants and head production. Parameters were more recently updated with more
    data
//double B = 8.71; //updated parameters from Integrated Management of Herbicide
    Resistance By S.R.Moss1, L.V.Tatnell12, R.Hull11, J.H.Clarke2, S.Wynn2 &
    R.Marshall11.
//double a = 0.005741;
//parameters for curve based on soil . Calculated for data from Metcalfe et al
    (life cycle chapter)
x1 = 844.4883;
x2 = 6.9542;
x3 = -106.7242;
double asy = 8.71 / 0.005741; //the asymptote remains the same as in the
    original work
```

```
// Calculate number of heads in each grid cell using a density dependent
function
double myslope = x1*myOm / (1 + x2*myOm) + x3;
double a = myslope / (asy - myslope);
double B = asy*a;

Heads = B*aPlants / (1 + a*aPlants);

//The yield of the black-grass plant will also respond to water stress
accumulated from germination to flowering
double yearend = 364;
myWater = Grid::GetSWC(irow, jcol);
averageVWC(irow, jcol, myWater, cultivationday, yearend, EarlysumVWC,
Earlycountdays);//accumulate available water for this part of the year
Grid::SetEarlySumVWC(irow, jcol, EarlysumVWC);
Grid::SetSWC(irow, jcol, myWater);//Set soil water for the year end
}

void growlate(int irow, int jcol, double& dropSeeds, double& aPlants, int
Earlycountdays, double Heads, int& harvestday, int flowerday, double LatesumVWC,
int Latecountdays)
// grow late continues the life-cycle from the endpoint of grow early. Now we have
the next years weather data. It runs from the start of the calendar year to
harvest.
// Inputs are the field size, the dates for harvest and flowering.
// Outputs are the number of plants in each cell and the amount of water
accumulated over this period
{
double yearstart = 0;

double myWater = Grid::GetSWC(irow, jcol); //Get water for yearstart
averageVWC(irow, jcol, myWater, yearstart, flowerday, LatesumVWC,
Latecountdays);//accumulate available water from the year start to flowering
Grid::SetSWC(irow, jcol, myWater);//Set soil water for flowerday
double EarlySumVWC = Grid::GetEarlySumVWC(irow, jcol);
double avgVWC = (EarlySumVWC + LatesumVWC) / (Earlycountdays +
Latecountdays);//This is the average VWC from germination to flowering

//compare this to field capacity and wilting point for that cell
double myw50, myw15000;
double mbar = 50;
vanGenuchten2(irow, jcol, mbar, myw50); //calculate water content needed for
mbar=50 (field capacity)
mbar = 15000;
vanGenuchten2(irow, jcol, mbar, myw15000); //calculate water content needed for
mbar=1500 (wilting point)

double propavailwater = (avgVWC - myw15000) / (myw50 - myw15000);//calculate
the proportion of available water experienced by the plant
Grid::Setpropavailablewater(irow, jcol, propavailwater);
double transp = 1 / (1 + 6.88*exp(-4.61*propavailwater));//Proportion of
potentail transpiration for BG from Storkey and Cussans 2007
Heads = Heads*transp;//Number of heads is reduced by a proportion that is
related to water stress
Grid::SetHeads(irow, jcol,Heads);//Set the number of heads to the grid - - This
```

```
    can be compared to summer head counts in the field
//
// *****/
//
// pSeeds is the number of seeds produced per head. Using the mean and 95%
// confidence intervals (given as range) in Moss(1990) a lognormal distribution
// is used to describe the germination rates.
double Mpseeds = 4.5779; // mean of lognormal for pSeeds
double Spseeds = 0.2337; // st dev of lognormal for pSeeds

// Calculate the number of seeds per head by taking numbers from a normal
// distribution
double Mu = Mpseeds; // mean of the normal distribution
double Var = Spseeds*Spseeds; //variance of the normal distribution

//This sets up the nag functions to calculate the selection of a random number
// from a normal distribution
int const LR = 1;
double R[LR];
double X[1];
int ifail = 1;
int const genid(1);
int const subid(0);
int lstate(17);
int* state; //when we declare 'state' we dont say how long it will be so we
// need to delete it after we have used it
state = new int[lstate]; //here we declare state again so must delete it again
ifail = 1;
G05KGF(genid, subid, state, lstate, ifail); //this is a non-repeatable seed
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05KGF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
int N = 1; // number of numbers to generate
G05SKF(N, Mu, Var, state, X, ifail); //Take the number of seeds from the
// distribution
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05SKF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
double SeedHeads = X[0];
SeedHeads = exp(SeedHeads); //because it is a lognormal distribution
SeedHeads = fmax(0, SeedHeads); // The number of seeds per head is limited to a
// minimum of 0

double TotalSeeds = Heads * SeedHeads; // The total number of seeds in the
```

```

    cell is calculated

    // vSeeds is the proportion of seeds that are viable. Using the mean and 95% ↗
    // confidence intervals (given as range) in Moss(1990) a normal distribution is ↗
    // used to describe the germination rates.
    double Mvseeds = 0.55; // mean of normal for vSeeds
    double Svseeds = 0.126; // st dev of normal for vSeeds

    Mu = Mvseeds; // mean of the normal distribution
    Var = Svseeds*Svseeds; //variance of the normal distribution

    G05SKF(N, Mu, Var, state, X, ifail);
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05SKF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    double Via = X[0]; //Via is the seed viability proportion

    Via = fmax(0, Via); // The proportion is limited to values between 0 and 1
    Via = fmin(1, Via);
    double viableSeeds = TotalSeeds * Via; // The number of viable seeds in the ↗
    // cell is calculated by multiplying the number of seeds by the viability ↗
    // proportion.

    // sSeeds is the proportion of seeds remaining after losses. Using the mean and ↗
    // 95% confidence intervals (given as range) in Moss(1990) a lognormal ↗
    // distribution is used to describe the germination rates.
    double Msseeds = -0.8070; // mean of lognormal for sSeeds
    double Ssseeds = 0.1303; // st dev of lognormal for vSeeds

    Mu = Msseeds; // mean of the lognormal distribution
    Var = Ssseeds*Ssseeds; //variance of the lognormal distribution
    G05SKF(N, Mu, Var, state, X, ifail);
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05SKF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    double Surv = X[0]; // Seed losses are calculated by selecting a survival % ↗
    // from a lognormal ↗
    // distribution
    Surv = exp(Surv);
    Surv = fmax(0, Surv); // The proportion is limited to values between 0 and 1
    Surv = fmin(1, Surv);

    dropSeeds = Surv * viableSeeds; // The number of seeds that are dropped by the ↗
    // plant and survive is calculated by multiplying the numebr of viable seeds by ↗
    // the survival proportion

```

```

//Calculate water deficit from flowering to harvest - used in germination next
season
double mydeficit = 0;

myWater = Grid::GetSWC(irow, jcol); //get the water stored in the grid for
flowerday
waterdeficit(irow, jcol, myWater, flowerday, harvestday, mydeficit); //calculate
the water deficit from flowering to harvest (this is needed in the
germination calculations)
Grid::SetWD(irow, jcol, mydeficit); //set water deficit to the grid for season
prior to model start
Grid::SetSWC(irow, jcol, myWater); //set soil water content at harvest to the
grid

Grid::SetDropSeeds(irow, jcol, dropSeeds); //set the number of seeds dropped
Grid::SetPlants(irow, jcol, aPlants); //set the number of mature plants
}

void Disp(std::vector<double>& proportions) //The Disp function uses the proportions
found in natDisp and allocates seeds to their new grid squares
{
    Grid::ClearTempWeeds();

    for (int icount = 0; icount < Grid::GetNumRows(); icount++) //go through each
grid cell in turn
    {
        for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
        {
            int numSeeds = int(round(Grid::GetDropSeeds(icount, jcount))); //get
the number of Dropped seeds from plants in this cell
            Distribute2(icount, jcount, proportions, numSeeds); //distribute those
seeds using function Distribute2 in Grow.cpp. These are now in
TempWeeds
        }
    }
}

void Distribute2(int irow, int jcol, std::vector<double>& proportions, int
numseeds) //This function distributes the seeds according to binomial with
parameter gamma and nu
{
    if (numseeds == 0) //if there are no seeds don't worry
    {
        return;
    }
    else
    {
        double P_Sum = 0; // to keep track of probability used so that we readjust
        int numSum = 0;
        int NRows = Grid::GetNumRows();
        int NCols = Grid::GetNumCols();
        int Len = proportions.size();
    }
}

```

```

//central point

double NewV(0);

int N = 1;
int M = numseeds;

//The probability of landing in cell irow, jcol
double P = proportions[0];

//
*****
***//
//This sets up the nag functions to calculate the binomial outcome from
numseeds events and P prob
int const LR = 1;
double R[LR];
int X[1];
int ifail = 1;
int MODE = 3;
int const genid(1);
int const subid(0);
int lstate(17);
int* state; //when we declare 'state' we dont say how long it will be so we
need to delete it after we have used it
state = new int[lstate];
ifail = 1;
G05KGF(genid, subid, state, lstate, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05KGF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
G05TAF(MODE, N, M, P, R, LR, state, X, ifail); //The number of seeds that
fall is X
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}

//
*****
***//
//From a crop competition model by AE Milne//
P_Sum = P_Sum + proportions[0];
M = M - X[0];

//Add into temporary weed structure
NewV = Grid::GetTempWeed(irow, jcol) + X[0]; //The weeds that were in

```

```
    centre cell + new dropped seeds
    Grid::SetTempWeed(irow, jcol, NewV);
    numSum = numSum + X[0]; //number of seeds that have dropped so far

    int sideCount(2);
    int LenCount(3);
    while (Len>LenCount - 1) //next square%
    {
        //sides
        int nrow = irow;
        int ncol = jcol + sideCount - 1;
        Reflect(nrow, ncol); //reflects seeds back into the field

        if (P_Sum < 1)
        {
            P = (proportions[LenCount - sideCount]) / (1 - P_Sum);
        }
        else
        {
            P = 1;
        }
        if (P>1)
            P = 1;
        G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
        if (ifail != 0)
        {
            char myText[10];
            _itoa_s(ifail, myText, 10);
            char myBigText[50] = " Error in Nag G05TAF ";
            strcat_s(myBigText, myText);
            throw std::logic_error(myBigText);
        }
        P_Sum = P_Sum + proportions[LenCount - sideCount];
        M = M - X[0];

        if (X[0] > 0)
        {
            NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
            Grid::SetTempWeed(nrow, ncol, NewV);
            numSum = numSum + X[0];
        }

        nrow = irow;
        ncol = jcol - sideCount + 1;
        Reflect(nrow, ncol);

        if (P_Sum < 1)
        {
            P = (proportions[LenCount - sideCount]) / (1 - P_Sum);
        }
        else
        {
            P = 1;
        }
        if (P>1)
            P = 1;
    }
}
```

```
G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
P_Sum = P_Sum + proportions[LenCount - sideCount];
M = M - X[0];

if (X[0] > 0)
{
    NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
    Grid::SetTempWeed(nrow, ncol, NewV);
    numSum = numSum + X[0];
}

nrow = irow + sideCount - 1;
ncol = jcol;
Reflect(nrow, ncol);

if (P_Sum < 1)
{
    P = (proportions[LenCount - sideCount]) / (1 - P_Sum);
}
else
{
    P = 1;
}
if (P>1)
    P = 1;
G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
P_Sum = P_Sum + proportions[LenCount - sideCount];
M = M - X[0];

if (X[0] > 0)
{
    NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
    Grid::SetTempWeed(nrow, ncol, NewV);
    numSum = numSum + X[0];
}

nrow = irow - sideCount + 1;
ncol = jcol;
Reflect(nrow, ncol);
```

```

if (P_Sum < 1)
{
    P = (proportions[LenCount - sideCount]) / (1 - P_Sum);
}
else
{
    P = 1;
}
if (P>1)
    P = 1;
G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
P_Sum = P_Sum + proportions[LenCount - sideCount];
M = M - X[0];

if (X[0] > 0)
{
    NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
    Grid::SetTempWeed(nrow, ncol, NewV);
    numSum = numSum + X[0];
}

//corners

nrow = irow + sideCount - 1;
ncol = jcol + sideCount - 1;
Reflect(nrow, ncol);

if (P_Sum < 1)
{
    P = (proportions[LenCount - 1]) / (1 - P_Sum);
}
else
{
    P = 1;
}
if (P>1)
    P = 1;
G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}

```

```
}
P_Sum = P_Sum + proportions[LenCount - 1];
M = M - X[0];
if (X[0] > 0)
{
    NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
    Grid::SetTempWeed(nrow, ncol, NewV);
    numSum = numSum + X[0];
}

nrow = irow + sideCount - 1;
ncol = jcol - sideCount + 1;
Reflect(nrow, ncol);

if (X[0] > 0)
{
    if (P_Sum < 1)
    {
        P = (proportions[LenCount - 1]) / (1 - P_Sum);
    }
    else
    {
        P = 1;
    }
}
if (P > 1)
    P = 1;
G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
P_Sum = P_Sum + proportions[LenCount - 1];
M = M - X[0];
if (X[0] > 0)
{
    NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
    Grid::SetTempWeed(nrow, ncol, NewV);
    numSum = numSum + X[0];
}

nrow = irow - sideCount + 1;
ncol = jcol + sideCount - 1;
Reflect(nrow, ncol);

if (P_Sum < 1)
{
```

```
        P = (proportions[LenCount - 1]) / (1 - P_Sum);
    }
    else
    {
        P = 1;
    }
    if (P>1)
        P = 1;
    G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05TAF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    P_Sum = P_Sum + proportions[LenCount - 1];
    M = M - X[0];
    if (X[0] > 0)
    {
        NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
        Grid::SetTempWeed(nrow, ncol, NewV);
        numSum = numSum + X[0];
    }

    nrow = irow - sideCount + 1;
    ncol = jcol - sideCount + 1;
    Reflect(nrow, ncol);

    if (P_Sum < 1)
    {
        P = (proportions[LenCount - 1]) / (1 - P_Sum);
    }
    else
    {
        P = 1;
    }
    if (P>1)
        P = 1;
    G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05TAF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    P_Sum = P_Sum + proportions[LenCount - 1];
    M = M - X[0];
    if (X[0] > 0)
    {
```

```

        NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
        Grid::SetTempWeed(nrow, ncol, NewV);
        numSum = numSum + X[0];
    }
    //diagonalsides

    int Mid = sideCount - 2;

    for (int Mcount = 0; Mcount<Mid; Mcount++)
    {
        nrow = irow + Mcount + 1;
        ncol = jcol + sideCount - 1;
        Reflect(nrow, ncol);

        if (P_Sum < 1)
        {
            P = (proportions[LenCount - sideCount + Mcount + 1]) / (1 - P_Sum);
        }
        else
        {
            P = 1;
        }

        if (P>1)
            P = 1;

        G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
        if (ifail != 0)
        {
            char myText[10];
            _itoa_s(ifail, myText, 10);
            char myBigText[50] = " Error in Nag G05TAF ";
            strcat_s(myBigText, myText);
            throw std::logic_error(myBigText);
        }
        P_Sum = P_Sum + proportions[LenCount - sideCount + Mcount + 1];
        M = M - X[0];
        if (X[0] > 0)
        {

            NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
            Grid::SetTempWeed(nrow, ncol, NewV);
            numSum = numSum + X[0];
        }

        nrow = irow - Mcount - 1;
        ncol = jcol + sideCount - 1;
        Reflect(nrow, ncol);

        if (P_Sum < 1)
        {
            P = (proportions[LenCount - sideCount + Mcount + 1]) / (1 - P_Sum);
        }
    }

```

```
else
{
    P = 1;
}
if (P>1)
    P = 1;

G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
P_Sum = P_Sum + proportions[LenCount - sideCount + Mcount + 1];
M = M - X[0];
if (X[0] > 0)
{

    NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
    Grid::SetTempWeed(nrow, ncol, NewV);
    numSum = numSum + X[0];

}

nrow = irow + Mcount + 1;
ncol = jcol - sideCount + 1;
Reflect(nrow, ncol);

if (P_Sum < 1)
{
    P = (proportions[LenCount - sideCount + Mcount + 1]) / (1 - P_Sum);
}
else
{
    P = 1;
}
if (P>1)
    P = 1;

G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
P_Sum = P_Sum + proportions[LenCount - sideCount + Mcount + 1];
M = M - X[0];
if (X[0] > 0)
```

```

    {

        NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
        Grid::SetTempWeed(nrow, ncol, NewV);
        numSum = numSum + X[0];

    }

    nrow = irow - Mcount - 1;
    ncol = jcol - sideCount + 1;
    Reflect(nrow, ncol);

    if (P_Sum < 1)
    {
        P = (proportions[LenCount - sideCount + Mcount + 1]) / (1 - P_Sum);
    }
    else
    {
        P = 1;
    }
    if (P>1)
        P = 1;

    G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05TAF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    P_Sum = P_Sum + proportions[LenCount - sideCount + Mcount + 1];
    M = M - X[0];
    if (X[0] > 0)
    {

        NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
        Grid::SetTempWeed(nrow, ncol, NewV);
        numSum = numSum + X[0];

    }

    ////
    nrow = irow + sideCount - 1;
    ncol = jcol + Mcount + 1;
    Reflect(nrow, ncol);

    if (P_Sum < 1)
    {
        P = (proportions[LenCount - sideCount + Mcount + 1]) / (1 - P_Sum);
    }
    else
    {

```

```
        P = 1;
    }
    if (P>1)
        P = 1;

    G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05TAF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    P_Sum = P_Sum + proportions[LenCount - sideCount + Mcount + 1];
    M = M - X[0];
    if (X[0] > 0)
    {

        NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
        Grid::SetTempWeed(nrow, ncol, NewV);
        numSum = numSum + X[0];

    }

    nrow = irow + sideCount - 1;
    ncol = jcol - Mcount - 1;
    Reflect(nrow, ncol);

    if (P_Sum < 1)
    {
        P = (proportions[LenCount - sideCount + Mcount + 1]) / (1 - P_Sum);
    }
    else
    {
        P = 1;
    }
    if (P>1)
        P = 1;

    G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05TAF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    P_Sum = P_Sum + proportions[LenCount - sideCount + Mcount + 1];
    M = M - X[0];

    if (X[0] > 0)
    {
```

```
NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
Grid::SetTempWeed(nrow, ncol, NewV);
    numSum = numSum + X[0];

}

nrow = irow - sideCount + 1;
ncol = jcol + Mcount + 1;
Reflect(nrow, ncol);

if (P_Sum < 1)
{
    P = (proportions[LenCount - sideCount + Mcount + 1]) / (1 - P_Sum);
}
else
{
    P = 1;
}
if (P>1)
    P = 1;

G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
P_Sum = P_Sum + proportions[LenCount - sideCount + Mcount + 1];
M = M - X[0];
if (X[0] > 0)
{

    NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
    Grid::SetTempWeed(nrow, ncol, NewV);
        numSum = numSum + X[0];

}

nrow = irow - sideCount + 1;
ncol = jcol - Mcount - 1;
Reflect(nrow, ncol);

if (P_Sum < 1)
{
    P = (proportions[LenCount - sideCount + Mcount + 1]) / (1 - P_Sum);
}
else
{
    P = 1;
}
if (P>1)
```

```

        P = 1;
        G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
        if (ifail != 0)
        {
            char myText[10];
            _itoa_s(ifail, myText, 10);
            char myBigText[50] = " Error in Nag G05TAF ";
            strcat_s(myBigText, myText);
            throw std::logic_error(myBigText);
        }
        P_Sum = P_Sum + proportions[LenCount - sideCount + Mcount + 1];
        M = M - X[0];
        if (X[0] > 0)
        {
            NewV = Grid::GetTempWeed(nrow, ncol) + X[0];
            Grid::SetTempWeed(nrow, ncol, NewV);
            numSum = numSum + X[0];
        }

    }

    sideCount++; //these keep track of where you are on square
    LenCount = LenCount + sideCount;

}
delete[] state;
state = NULL;
if (numSum < numseeds)
{
    NewV = Grid::GetTempWeed(irow, jcol) + numseeds - numSum;
    Grid::SetTempWeed(irow, jcol, NewV);
}
}

}

void natDisp(std::vector<double>& Type, double& extra, double mu, double sigma) ↗

//This is a function that reads in the information about the natural dispersal ↗
parameters and integrates cells under the curve to determine the proportion of ↗
seeds which will be dispersed into different cell types.
//Outputs are a list of proportions to move to each cell type and the remaining ↗
proportion that is not currently allocated to any cell type
{

    int idist = 0;
    int jdist = 0;

    Type.push_back(Integrate(idist, jdist, mu, sigma)); //position 0

```

```

Type.push_back(Integrate(0, 1, mu, sigma)); //position 1
Type.push_back(Integrate(1, 1, mu, sigma)); //position 2
//Test to see how much of the population is in this inner square
double popT = Type[0] + 4 * Type[1] + 4 * Type[2];
//if (popT<0.99) //keep calculating
int Mcount = 3;
while (popT<0.999)
{
    for (int icount = 0; icount<Mcount; icount++)
    {
        double Ival = Integrate(icount, Mcount - 1, mu, sigma);
        Type.push_back(Ival);
        if ((icount>0) && (icount < Mcount - 1))
        {
            popT = popT + 8 * Ival;
            if (popT > 1)
            {
                double rem = popT - 1;
                int len = Type.size();
                Type[len - 1] = Type[len - 1] - rem / 8;
                popT = 1;
            }
        }
        else
        {
            popT = popT + 4 * Ival;
            if (popT > 1)
            {
                double rem = popT - 1;
                int len = Type.size();
                Type[len - 1] = Type[len - 1] - rem / 4;
                popT = 1;
            }
        }
    }
    Mcount++;
}
//put remained in extra
extra = 1.0 - popT;
}

double Integrate(int idist, int jdist, double mu, double sigma)
{
    //This function integrates the dispersal distributions over each cell.
    //inputs are the mean and stdev of the distribution
    //By AE Milne

    double gridLen = Grid::GetCell(); // get the size of a grid cell

    Grid::SetIntVars(mu, sigma);

```

```

double xlb[2], xub[2];
xlb[0] = (idist - 0.5)*gridLen;
xlb[1] = (jdist - 0.5)*gridLen;
xub[0] = (idist + 0.5)*gridLen;
xub[1] = (jdist + 0.5)*gridLen;

double ABSACC = 0.0;
double RELACC = 0.0000001;

int NDIM(2);
int NumFunc(1);
int MaxCals(18000000);
int MinCals(10);
const int LENWRK = 500;
double WRKSTR[LENWRK];
int IFAIL = 1;
double ANS[1];
double ABSET[1];

D01EAF(NDIM, xlb, xub, MinCals, MaxCals, NumFunc, fFunc2, ABSACC, RELACC,
      LENWRK, WRKSTR, ANS, ABSET, IFAIL);

if (ANS[0]<0)
    throw std::logic_error("Error in integration");
if (IFAIL != 0)
    int junk = 0;

return ANS[0];
}

extern "C" void __stdcall fFunc2(const int& NDIM, const double x[], const int&
      NumFunc, double funcY[])
{
    //Rotated Gaussian function from Paice et al 1998 predicts the distribution
    // of seeds released from plants in the starting cell

    double mu, sigma;
    Grid::GetIntVars(mu, sigma);
    int IFAIL = 1;

    double func(0);
    double OOtwoPi = 1.0 / (2.0*3.141572);

    func = OOtwoPi/(sigma*sigma)*exp(-0.5*(((x[0] - mu) / sigma)*((x[0] - mu) /
      sigma) + ((x[1] - mu) / sigma)*((x[1] - mu) / sigma)));
    funcY[0] = func;
}

void Reflect(int& nrow, int& ncol)//put seeds back into field if they are dispersed
      outside of the field boundary
{
    int NRows = Grid::GetNumRows();

```

```
int NCols = Grid::GetNumCols();
while ((nrow>NRows - 1) || (nrow<0))
{
    if (nrow<0)
    {
        nrow = -1 - nrow;
    }
    else if (nrow>NRows - 1)
    {
        nrow = 2 * NRows - 1 - nrow;
    }
}
while ((ncol>NCols - 1) || (ncol<0))
{
    if (ncol<0)
    {
        ncol = -1 - ncol;
    }
    else if
        (ncol>NCols - 1)
    {
        ncol = 2 * NCols - 1 - ncol;
    }
}
}

void WritePlants(int iyr)//create a text file in outputs with the numebr of plants ↗
in the given year
{
    char path_buffer[_MAX_PATH];
    char Npath_buffer[_MAX_PATH];
    _getcwd(path_buffer, _MAX_PATH);
    strcpy_s(Npath_buffer, path_buffer);

    char Crop[50];
    int n = sprintf_s(Crop, 50, "\\OutFiles\\Plants%d.txt", iyr);
    strcat_s(Npath_buffer, Crop);
    std::ofstream OutF(Npath_buffer);

    if (OutF)
    {
        for (int jcount = 0; jcount<Grid::GetNumRows(); jcount++)
        {
            for (int icount = 0; icount<Grid::GetNumCols(); icount++)
            {
                OutF << Grid::GetPlants(jcount, icount) << '\t'; //'\t' is a tab ↗
                between numbers
            }
            OutF << '\n'; //'\n' is a line return
        }
    }
}
```

```
    else
        throw std::logic_error("Error in write plants");
}

void WriteSWC(int iyr)//create a text file in outputs with the SWC in the given year
{
    char path_buffer[_MAX_PATH];
    char Npath_buffer[_MAX_PATH];
    _getcwd(path_buffer, _MAX_PATH);
    strcpy_s(Npath_buffer, path_buffer);

    char Crop[50];
    int n = sprintf_s(Crop, 50, "\\OutFiles\\SWC%d.txt", iyr);
    strcat_s(Npath_buffer, Crop);
    std::ofstream OutF(Npath_buffer);

    if (OutF)
    {
        for (int jcount = 0; jcount<Grid::GetNumRows(); jcount++)
        {
            for (int icount = 0; icount<Grid::GetNumCols(); icount++)
            {
                OutF << Grid::GetSWC(jcount, icount) << '\t'; //'\t' is a tab
                    between numbers
            }
            OutF << '\n'; //'\n' is a line return
        }
    }
    else
        throw std::logic_error("Error in write plants");
}

void Writepropavailablewater(int iyr)//create a text file in outputs with the
proportion of available water in the given year
{
    char path_buffer[_MAX_PATH];
    char Npath_buffer[_MAX_PATH];
    _getcwd(path_buffer, _MAX_PATH);
    strcpy_s(Npath_buffer, path_buffer);

    char Crop[50];
    int n = sprintf_s(Crop, 50, "\\OutFiles\\propavailablewater%d.txt", iyr);
    strcat_s(Npath_buffer, Crop);
    std::ofstream OutF(Npath_buffer);

    if (OutF)
    {
        for (int jcount = 0; jcount<Grid::GetNumRows(); jcount++)
        {
```

```

        for (int icount = 0; icount<Grid::GetNumCols(); icount++)
        {
            OutF << Grid::Getpropavailablewater(jcount, icount) << '\t'; //'t' is a tab between numbers
        }
        OutF << '\n'; //'t' is a line return
    }
}
else
    throw std::logic_error("Error in write propavailablewater");
}

```

```

void WriteSeedlings(int iyr)//create a text file in outputs with the number of seedlings in the given year

```

```

{
    char path_buffer[_MAX_PATH];
    char Npath_buffer[_MAX_PATH];
    _getcwd(path_buffer, _MAX_PATH);
    strcpy_s(Npath_buffer, path_buffer);

    char Crop[50];
    int n = sprintf_s(Crop, 50, "\\OutFiles\\Seedlings%d.txt", iyr);
    strcat_s(Npath_buffer, Crop);
    std::ofstream OutF(Npath_buffer);
    if (OutF)
    {
        for (int jcount = 0; jcount<Grid::GetNumRows(); jcount++)
        {
            for (int icount = 0; icount<Grid::GetNumCols(); icount++)
            {
                OutF << Grid::GetSeedlings(jcount, icount) << '\t'; //'t' is a tab between numbers
            }
            OutF << '\n'; //'t' is a line return
        }
    }
    else
        throw std::logic_error("Error in write seedlings");
}

```

```

void WriteHeads(int iyr)//create a text file in outputs with the number of heads in the given year

```

```

{
    char path_buffer[_MAX_PATH];
    char Npath_buffer[_MAX_PATH];
    _getcwd(path_buffer, _MAX_PATH);
    strcpy_s(Npath_buffer, path_buffer);

    char Crop[50];
    int n = sprintf_s(Crop, 50, "\\OutFiles\\Heads%d.txt", iyr);
    strcat_s(Npath_buffer, Crop);
    std::ofstream OutF(Npath_buffer);
}

```

```

if (OutF)
{
    for (int jcount = 0; jcount<Grid::GetNumRows(); jcount++)
    {
        for (int icount = 0; icount<Grid::GetNumCols(); icount++)
        {
            OutF << Grid::GetHeads(jcount, icount) << '\t'; //'t' is a tab ↗
                between numbers
        }
        OutF << '\n'; //'t' is a line return
    }
}
else
    throw std::logic_error("Error in write heads");
}
void soilMove(int iYear, int cult)
{
    // soilMove is a function that relocates seeds within the seed bank to ↗
    // different depths according to the cultivation method in use.
    // Inputs are the number of old and new seeds currently at both depths in the ↗
    // soil, the dispersed seeds from the current year,
    // the cultivation type, the field size and the year.
    // Outputs are the number of old and new seeds currently at both depths in the ↗
    // soil.

    //This sets up the nag functions to calculate the selection of a random number ↗
    // from a normal distribution
    int const LR = 1;
    double R[LR];
    double X[1];
    int ifail = 1;
    int const genid(1);
    int const subid(0);
    int lstate(17);
    int* state; //when we declare 'state' we dont say how long it will be so we ↗
    // need to delete it after we have used it

    state = new int[lstate]; //here we declare state again so must delete it again
    ifail = 1;
    G05KGF(genid, subid, state, lstate, ifail); //this is a non-repeatable seed
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05KGF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    int N = 1; // number of numbers to generate

    //***** /

    /*Function parameters
    The parameters required by the model to run, can be altered to

```

```

investigate different scenarios

soilSurv is the survival rate of seeds in the soil.Using the mean and
95 % confidence intervals(given as range) in Moss(1990) a normal
distribution is used. */
double MsoilSurv, SsoilSurv, SoilSurv;
MsoilSurv = 0.3; // Mean of normal for soilSurv
SsoilSurv = 0.077; // St dev of normal for soilSurv

double Mu = MsoilSurv; // mean of the normal distribution
double Var = SsoilSurv*SsoilSurv; //variance of the normal distribution

G05SKF(N, Mu, Var, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05SKF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
SoilSurv = X[0];
SoilSurv = fmax(0, SoilSurv); //The proportion is limited to values between 0
and 1
SoilSurv = fmin(1, SoilSurv);

/*c1Bury is the proportion of seeds that are buried with cultivation type 1
Using the mean and 95 % confidence intervals(given as range) in
Moss(1990) a lognormal distribution is fitted.*/
double c1Bury, sB1, c1bRand;
c1Bury = -0.0515; //Mean of lognormal for c1Bury
sB1 = 0.0191; //st dev of lognormal for c1Bury
Mu = c1Bury;
Var = sB1*sB1;
G05SKF(N, Mu, Var, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05SKF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
c1bRand = X[0];
c1bRand = exp(c1bRand);
c1bRand = fmax(0, c1bRand); // The proportion is limited to values between 0
and 1
c1bRand = fmin(1, c1bRand);

/*c2Bury is the proportion of seeds that are buried with cultivation type 2*/
double c2Bury=0;
//c2Bury = zeros(nrows, ncols); /* As no seeds are buried there is no need to
// generate a distribution*/

/* c3Bury is the proportion of seeds that are buried with cultivation type 3
Using the mean and 95 % confidence intervals(given as range) in

```

```

    Moss(1990) a normal distribution is fitted.*/
double c3Bury, sB3, c3bRand;
c3Bury = 0.2; // Mean of normal for c3Bury
sB3 = 0.051; // st dev of normal for c3Bury
Mu = c3Bury;
Var = sB3*sB3;
G05SKF(N, Mu, Var, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05SKF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
c3bRand = X[0];
c3bRand = fmax(0, c3bRand); //The proportion is limited to values between 0 and 1
c3bRand = fmin(1, c3bRand);

/* c4Bury is the proportion of seeds that are buried with cultivation type 4
Using the mean and 95 % confidence intervals(given as range) in
Moss(1990) a normal distribution is fitted.*/
double c4Bury, sB4, c4bRand;
c4Bury = 0.4; // Mean of normal for c4Bury
sB4 = 0.101; // st dev of normal for c4Bury
Mu = c4Bury;
Var = sB4*sB4;
G05SKF(N, Mu, Var, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05SKF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
c4bRand = X[0];
c4bRand = fmax(0, c4bRand); // The proportion is limited to values between 0 and 1
c4bRand = fmin(1, c4bRand);

/* c1Rise is the proportion of seeds that rise with cultivation type 1
%% Using the mean and 95 % confidence intervals(given as range) in
% Moss(1990) a lognormal distribution is fitted.*/
double c1Rise, sR1, c1rRand;
c1Rise = -1.0570; //Mean of lognormal for c1Rise
sR1 = 0.1199; //st dev of lognormal for c1Rise
Mu = c1Rise;
Var = sR1*sR1;
G05SKF(N, Mu, Var, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05SKF ";

```

```

        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    c1rRand = X[0];
    c1rRand = exp(c1rRand);
    c1rRand = fmax(0, c1rRand); // The proportion is limited to values between ↗
    0 and 1
    c1rRand = fmin(1, c1rRand);

    /* c2Rise is the proportion of seeds that rise with cultivation type 2*/
    double c2Rise=0; // As no seeds are buried there is no need to generate a ↗
    distribution

    /*c3Rise is the proportion of seeds that rise with cultivation type 3*/
    double c3Rise=0; // As no seeds are buried there is no need to generate a ↗
    distribution

    /*c4Rise is the proportion of seeds that rise with cultivation type 4*/
    double c4Rise=0; // As no seeds are buried there is no need to generate a ↗
    distribution

    delete[] state;
    // Create cell arrays to store the proportions of seeds that are buried and ↗
    rise according to cultivation type.
    //The index cult, assigned in Weeds_2.cpp tells which position in the array ↗
    to use for each year
    double bury[4] = { c1bRand, c2Bury, c3bRand, c4bRand };
    double rise[4] = { c1rRand, c2Rise, c3Rise, c4Rise };

    //For each row and column bury seeds and bring them up according to the ↗
    cultivation type
    for (int icount = 0; icount < Grid::GetNumRows(); icount++)
    {
        for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
        {
            /* Seed Movement in the soil
            Seeds are moved between the soil layers according to the ↗
            cultivation type
            that year*/
            double myOldSeeds[2], myNewSeeds[2];
            Grid::GetOldSeeds(icount, jcount, myOldSeeds);
            Grid::GetNewSeeds(icount, jcount, myNewSeeds);

            double OSS, OSD, NSS, NSD;
            OSS = myOldSeeds[0];
            OSD = myOldSeeds[1];
            NSS = myNewSeeds[0];
            NSD = myNewSeeds[1];

            /*All seeds in the surface layer become old and are subjected to ↗
            survival
            rates */
            OSS = (OSS + NSS)*SoilSurv;
            NSS = 0;
            /* All seeds in the deep layer become old and are subjected to ↗

```

```

        survival
        rates*/
        OSD = (NSD + OSD)*SoilSurv;
        NSD = 0;

        // The newly shed seeds that are buried are determined by indexing ↗
        // bury according to the cultivation type for that year
        //and multiplying the values by the newly dispersed seeds
        double dispSeeds = Grid::GetTempWeed(icount, jcount);
        NSD = dispSeeds*bury[cult];
        /*The new seeds that remain on teh surface are determined by the ↗
        number that were dispersed here minus those that were buried*/
        NSS = dispSeeds - NSD;

        //The old seeds in the deep soil layer are calculated by taking the ↗
        // old seeds in the surface that are buried
        //and the old seeds in the deep layer that do not rise and adding ↗
        // them together
        double burySeedsDeep = (OSS*(bury[ cult ]))+OSD*(1 - rise ↗
        [ cult ]));

        //The old seeds on the surface are calculated by adding together ↗
        // the old
        //seeds on teh surface that are not buried to the old seeds from ↗
        // the deep layer that rise
        OSS = OSS*(1 - bury[cult]) + OSD*rise[cult];
        OSD = burySeedsDeep;
        double myOSeeds[2] = { OSS, OSD };
        Grid::SetOldSeeds(icount, jcount, myOSeeds);
        double myNSeeds[2] = { NSS, NSD };
        Grid::SetNewSeeds(icount, jcount,myNSeeds );
    }
}

}

void cultDisp(std::vector<double>& proportions2, double& extra2, double lambda, ↗
double eta, double b)
//This is a function that reads in the information about the cultivation dispersal ↗
// parameters and integrates cells under the curve to determine the proportion of ↗
// seeds which will be dispersed into different cell types.
//Outputs are a list of proportions to move to each cell type and the remainng ↗
// proportion that is not currently allocated to any cell type
{
    double gamma = 1 / b; // Additional distribution parameters are calculated from ↗
    // the inputs
    double grid = Grid::GetCell();

    Grid::SetIntVarsCult(lambda, eta, gamma);

    // % Proportions will store the proportion of seeds that move to each cell ↗
    // % tProportion calculates the total proportion of seeds already accounted ↗
    // for

```

```

double tProportion = 0;

    ///% Integrate the function
    // % The integration is carried out for each set of coordinates in turn until
    // % the total proportion accounted for is >= 0.999
    int i = 1; ///% set a counter to 1. This will increment upon each      ↗
        integration and
    // % will allow reference to which cell type is currently being investigated
    int j = 2; ///%As the cultivation dispersal function goes in both direction ↗
        from
    // % the 0 starting point we need to consider both direction so a second      ↗
        counter is used to begin counting positions in the opposite direction
    double myIntVal(0);
    while (tProportion < 0.999) ///% whilst we still havent reached a total      ↗
        proportion ///% of seeds is <0.999 we should integrate at each position

    {
        ///% initially we will look at the proportion of seeds that travel in      ↗
            the opposite direction to the direction of travel up to a maximum of ↗
            5 grid squares
        if (i <= 5)
        {
            double xmin = -((grid*(i - 1)) + (grid / 2));
            double xmax = -((grid*(i - 2)) + (grid / 2));
            myIntVal = IntegrateCult(xmin, xmax);
            proportions2.push_back(myIntVal); ///% Integrate from xmin to xmax ↗
                according to the distance from the starting point in terms of ↗
                grid size
        }

        else ///% look at the proportion of seeds that travel various distances ↗
            in the direction of travel
        {
            double xmin = (grid*(j - 1)) - (grid / 2);
            double xmax = (grid*j) - (grid / 2);
            myIntVal = IntegrateCult(xmin, xmax);
            proportions2.push_back(myIntVal); ///% Integrate from xmin to xmax
                ///% according to the distance from the starting point in terms ↗
                of
                ///% grid size
            j = j + 1;
        }

        tProportion = tProportion + myIntVal;
        if (tProportion > 1)
        {
            double Remainder = tProportion - 1;
            proportions2[i - 1] = proportions2[i - 1] - Remainder;
        }

        // % if we have reached a total that is >1 subtract the excess from      ↗
            the
            // % last cell type to be integrated

            i = i + 1;/// % The counter is then incremented
    }
}

```

```

    extra2 = 1 - tProportion;
}

double IntegrateCult(double xmin, double xmax)
{
    //This function integrates the distributions over each cell .
    //By AE Milne

    double ABSACC = 0.0;
    double RELACC = 0.0000001;
    //double ANS(0);
    int NDIM(1);
    int NumFunc(1);
    int MaxCals(1800000);
    int MinCals(10);
    const int LENWRK = 500; //(NDIM+NumFunc+2)*(10+MaxCals);
    double WRKSTR[LENWRK];
    int IFAIL = 1;
    double ANS[1];
    double ABSET[1];

    //D01DAF(xlb, xub, ylbFunc, yubFunc, fFunc, ABSACC, ANS, NPTS, IFAIL);
    D01EAF(NDIM, &xmin, &xmax, MinCals, MaxCals, NumFunc, fFunc3, ABSACC, RELACC, ↗
        LENWRK, WRKSTR, ANS, ABSET, IFAIL);

    if (ANS[0]<0)
        throw std::logic_error("Error in integration");
    if (IFAIL != 0)
        int junk = 0;

    //ANS[0]=ANS[0]*ga;
    return ANS[0];
}

extern "C" void __stdcall fFunc3(const int& NDIM, const double x[], const int& ↗
    NumFunc, double funcY[])
//void fFunc2(const int& NDIM, const double x[], const int& NumFunc, double funcY ↗
[] )
{
    //Rotated Gaussian function from Paice et al 1998 predicts the distribution
    // of seeds released from plants in the starting cell

    double lambda, eta, gamma;
    Grid::GetIntVarsCult(lambda, eta, gamma);
    int IFAIL = 1;

    double func(0);
    double OOtwoPi = 1.0 / (2.0*3.141572);

    // In paice et al 1998 cultivator dispersal was described by a Gaussian ↗
    function and an exponential function

```

```

// z = @(x)(1. / (lambda.*(sqrt(2.*pi)))).*exp(-0.5.*((x - eta). / lambda). ^ 2);
// f = @(x)(b.*exp(-b.*x));

//Here an exponentially modified Gaussian distribution is described

double myerfcx = (eta + gamma*pow(lambda, 2) - x[0]) / (sqrt(2)*lambda);
double callerfc = S15ADF(myerfcx, IFAIL);

func = gamma / 2 * (exp((gamma / 2)*(2 * eta + gamma*pow(lambda, 2) - 2 * x
[0])))*callerfc;

funcY[0] = func;
}

void cdisp2NSS(std::vector<double> proportions2, double extra2, int maxd) //New
seeds shallow
//This is a function which moves seeds in the soil in the direction of cultivation
//Inputs are the proportions generated by integration of the cultural dispersal
distribution, the extra proportion from the integration and the maximum dispersal
distance.
//Output is the new numebr of seeds of the type of interest in the soil layer of
interest.
{
    Grid::ClearTempWeeds();
    double myNSeeds[] = { 0, 0 };

    // Disperse seeds //
    // Seeds are distributed from their starting point in the direction of travel
    according to the results of the integration of the cultivation dispersal
    distribution

    for (int icount = 0; icount<Grid::GetNumRows(); icount++) //For each row in
    turn decide if the cultivator is travelling east or west
    {
        double cWidth = Grid::GetCultWidth();
        double DirInd = floor(icount / cWidth); // If this is even we shall go East
        if odd west
        double myrem = remainder(DirInd, 2);

        if (myrem == 0)
        {
            for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
            {

                Grid::GetNewSeeds(icount, jcount, myNSeeds);
                int numSeeds = int(myNSeeds[0]);
                //cultmoveW Function
                cultmoveW(proportions2, numSeeds, icount, jcount, maxd);
                //Disperses the seeds in the soil in the correct direction for when
                cultivation is in a westerly direction
            }
        }
    }
}

```

```

    }
}
else
{
    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {

        Grid::GetNewSeeds(icount, jcount, myNSeeds);
        int numSeeds = int(myNSeeds[0]);
        // cultmoveE Function
        cultmoveE(proportions2, numSeeds, icount, jcount, maxd);
        // Disperses the seeds in the soil in the correct direction for
        when cultivation is in a easterly direction

    }
}
for (int icount = 0; icount < Grid::GetNumRows(); icount++)
{
    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {
        double myNSeedsShallow;
        double myNSeedsAll[] = { 0, 0 };
        Grid::GetNewSeeds(icount, jcount, myNSeedsAll);
        double myNSeedsDeep = myNSeedsAll[1];
        myNSeedsShallow = Grid::GetTempWeed(icount, jcount);
        myNSeeds[0] = myNSeedsShallow;
        myNSeeds[1] = myNSeedsDeep;
        Grid::SetNewSeeds(icount, jcount, myNSeeds);
    }
}
}
void cdisp2NSD(std::vector<double> proportions2, double extra2, int maxd)//New
seeds deep
//This is a function which moves seeds in the soil in the direction of cultivation
//Inputs are the proportions generated by integration of the cultural dispersal
distribution, the extra proportion from the integration and the maximum dispersal
distance.
//Output is the new numebr of seeds of the type of interest in the soil layer of
interest.
{
    Grid::ClearTempWeeds();
    double myNSeeds[] = { 0, 0 };

    // Disperse seeds //
    // Seeds are distributed from their starting point in the direction of travel
    according to the results of the integration of the cultivation dispersal
    distribution

    for (int icount = 0; icount<Grid::GetNumRows(); icount++) //For each row in
    turn decide if the cultivator is travelling east or west
    {

```

```

double cWidth = Grid::GetCultWidth();
double DirInd = floor(icount / cWidth); // If this is even we shall go East ↗
    if odd west
double myrem = remainder(DirInd, 2);

if (myrem == 0)
{
    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {

        Grid::GetNewSeeds(icount, jcount, myNSeeds);
        int numSeeds = int(myNSeeds[1]);
        //cultmoveW Function
        cultmoveW(proportions2, numSeeds, icount, jcount, maxd);
        //Disperses the seeds in the soil in the correct direction for when ↗
        cultivation is in a westerly direction

    }
}
else
{
    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {

        Grid::GetNewSeeds(icount, jcount, myNSeeds);
        int numSeeds = int(myNSeeds[1]);
        // cultmoveE Function
        cultmoveE(proportions2, numSeeds, icount, jcount,maxd);
        // Disperses the seeds in the soil in the correct direction for ↗
        when cultivation is in a easterly direction

    }
}
}
for (int icount = 0; icount < Grid::GetNumRows(); icount++)
{
    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {
        double myNSeedsShallow;
        double myNSeedsAll[] = { 0, 0 };
        Grid::GetNewSeeds(icount, jcount, myNSeedsAll);
        myNSeedsShallow = myNSeedsAll[0];
        double myNSeedsDeep = Grid::GetTempWeed(icount, jcount);
        myNSeeds[0] = myNSeedsShallow;
        myNSeeds[1] = myNSeedsDeep;
        Grid::SetNewSeeds(icount, jcount, myNSeeds);
    }
}
}

void cdisp2OSS(std::vector<double> proportions2, double extra2, int maxd)//old ↗
    seeds shallow
//This is a function which moves seeds in the soil in the direction of cultivation
//Inputs are the proportions generated by integration of the cultural dispersal ↗

```

```

distribution, the extra proportion from the integration and the maximum dispersal
distance.
//Output is the new numebr of seeds of the type of interest in the soil layer of
interest.
{
    Grid::ClearTempWeeds();
    double myOSeeds[] = { 0, 0 };

    // Disperse seeds //
    // Seeds are distributed from their starting point in the direction of travel
    according to the results of the integration of the cultivation dispersal
    distribution

    for (int icount = 0; icount<Grid::GetNumRows(); icount++) //For each row in
    turn decide if the cultivator is travelling east or west
    {
        double cWidth = Grid::GetCultWidth();
        double DirInd = floor(icount / cWidth); // If this is even we shall go East
        if odd west
        double myrem = remainder(DirInd, 2);

        if (myrem == 0)
        {
            for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
            {

                Grid::GetOldSeeds(icount, jcount, myOSeeds);
                int numSeeds = int(myOSeeds[0]);
                //cultmoveW Function
                cultmoveW(proportions2, numSeeds, icount, jcount, maxd);
                //Disperses the seeds in the soil in the correct direction for when
                cultivation is in a westerly direction
                myOSeeds[0] = numSeeds;

            }
        }
        else
        {
            for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
            {

                Grid::GetOldSeeds(icount, jcount, myOSeeds);
                int numSeeds = int(myOSeeds[0]);
                // cultmoveE Function
                cultmoveE(proportions2, numSeeds, icount, jcount,maxd);
                // Disperses the seeds in the soil in the correct direction for
                when cultivation is in a easterly direction
                myOSeeds[0] = numSeeds;

            }
        }
    }
}
for (int icount = 0; icount < Grid::GetNumRows(); icount++)
{

```

```

    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {
        double myOSeedsShallow;
        double myOSeedsAll[] = { 0, 0 };
        Grid::GetOldSeeds(icontains, jcount, myOSeedsAll);
        double myOSeedsDeep = myOSeedsAll[1];
        myOSeedsShallow = Grid::GetTempWeed(icontains, jcount);
        myOSeeds[0] = myOSeedsShallow;
        myOSeeds[1] = myOSeedsDeep;
        Grid::SetOldSeeds(icontains, jcount, myOSeeds);
    }
}

void cdisp2OSD(std::vector<double> proportions2, double extra2, int maxd) //old seeds deep
//This is a function which moves seeds in the soil in the direction of cultivation
//Inputs are the proportions generated by integration of the cultural dispersal distribution, the extra proportion from the integration and the maximum dispersal distance.
//Output is the new numebr of seeds of the type of interest in the soil layer of interest.
{
    Grid::ClearTempWeeds();
    double myOSeeds[] = { 0, 0 };

    // Disperse seeds //
    // Seeds are distributed from their starting point in the direction of travel according to the results of the integration of the cultivation dispersal distribution

    for (int icount = 0; icount < Grid::GetNumRows(); icount++) //For each row in turn decide if the cultivator is travelling east or west
    {
        double cWidth = Grid::GetCultWidth();
        double DirInd = floor(icontains / cWidth); // If this is even we shall go East if odd west
        double myrem = remainder(DirInd, 2);

        if (myrem == 0)
        {
            for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
            {
                Grid::GetOldSeeds(icontains, jcount, myOSeeds);
                int numSeeds = int(myOSeeds[1]);
                //cultmoveW Function
                cultmoveW(proportions2, numSeeds, icount, jcount, maxd);
                //Disperses the seeds in the soil in the correct direction for when cultivation is in a westerly direction
            }
        }
        else
        {

```

```

    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {

        Grid::GetOldSeeds(icount, jcount, myOSeeds);
        int numSeeds = int(myOSeeds[1]);
        // cultmoveE Function
        cultmoveE(proportions2, numSeeds, icount, jcount, maxd);
        // Disperses the seeds in the soil in the correct direction for
        // when cultivation is in a easterly direction
    }
}

for (int icount = 0; icount < Grid::GetNumRows(); icount++)
{
    for (int jcount = 0; jcount < Grid::GetNumCols(); jcount++)
    {
        double myOSeedsDeep;
        double myOSeedsAll[] = { 0, 0 };
        Grid::GetOldSeeds(icount, jcount, myOSeedsAll);
        double myOSeedsShallow = myOSeedsAll[0];
        myOSeedsDeep = Grid::GetTempWeed(icount, jcount);
        myOSeeds[0] = myOSeedsShallow;
        myOSeeds[1] = myOSeedsDeep;
        Grid::SetOldSeeds(icount, jcount, myOSeeds);
    }
}

}

void cultmoveE(std::vector<double> proportions2, int numseeds, int icount, int
    jcount, int maxd)
//move seeds by cultivation - cultivator moving east
{
    if (numseeds == 0) //if there are no seeds don't worry
    {
        return;
    }
    else
    {
        double P_Sum = 0; // to keep track of probability used so that we readjust
        int numSum = 0;
        int NRows = Grid::GetNumRows();
        int NCols = Grid::GetNumCols();
        int Len = proportions2.size();
        double NewV(0);
        int N = 1;
        int M = numseeds;

        for (int kcount = 0; kcount < Len; kcount++)
        {

            //The probability of landing in cell irow, jcol
            double P = proportions2[kcount];

```

```

//
*****
***** //
//This sets up the nag functions to calculate the binomial outcome
from numseeds events and P prob
int const LR = 1;
double R[LR];
int X[1];
X[0] = 0;
int ifail = 1;
int MODE = 3;
int const genid(1);
int const subid(0);
int lstate(17);
int* state; //when we declare 'state' we dont say how long it will
be so we need to delete it after we have used it

state = new int[lstate];
ifail = 1;
G05KGF(genid, subid, state, lstate, ifail);
if (ifail != 0)
{
char myText[10];
_itoa_s(ifail, myText, 10);
char myBigText[50] = " Error in Nag G05KGF ";
strcat_s(myBigText, myText);
throw std::logic_error(myBigText);
}
if (kcount == 0) // For the first value in the array the seeds will
be dispersed into the starting square
{
G05TAF(MODE, N, M, P, R, LR, state, X, ifail); //The number of
seeds that fall is X

if (ifail != 0)
{
char myText[10];
_itoa_s(ifail, myText, 10);
char myBigText[50] = " Error in Nag G05TAF ";
strcat_s(myBigText, myText);
throw std::logic_error(myBigText);
}
//
*****
***** //
P_Sum = P_Sum + proportions2[kcount];
M = M - X[0];
//Add into temporary weed structure
NewV = Grid::GetTempWeed(icount, jcount) + X[0]; //The weeds
that were in centre cell + new dropped seeds
Grid::SetTempWeed(icount, jcount, NewV);
numSum = numSum + X[0]; //number of seeds that have dropped so
far
}
else if (kcount > 0 && kcount <= 4)//For values of kcount from 1-4
seeds will be dispersed in the opposite direction to the

```

```
direction of travel
{
    int ii = icount;
    if (ii < 0)
    {
        ii = 0;
    }
    if (ii > NRows - 1)
    {
        ii = NRows - 1;
    }
    int jj = jcount - kcount;
    if (jj < 0)
    {
        jj = 0;
    }
    if (jj > NCols - 1)
    {
        jj = NCols - 1;
    }

    if (P < 1)
    {
        P = (proportions2[kcount]) / (1 - P_Sum);
    }
    else
    {
        P = 1;
    }
    if (P > 1)
    {
        P = 1;
    }

    G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05TAF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    P_Sum = P_Sum + proportions2[kcount];
    M = M - X[0];
    if (X[0] > 0)
    {
        NewV = Grid::GetTempWeed(ii, jj) + X[0];
        Grid::SetTempWeed(ii, jj, NewV);
        numSum = numSum + X[0];
    }
}
else //For values of k >4 seeds will be dispersed in the direction ↗
of travel
{
```

```
int ii = icount;
if (ii < 0)
{
    ii = 0;
}
if (ii > NRows - 1)
{
    ii = NRows - 1;
}
int jj = jcount + (kcount - 4);
if (jj < 0)
{
    jj = 0;
}
if (jj > NCols - 1)
{
    jj = NCols - 1;
}

if (P_Sum < 1)
{
    P = (proportions2[kcount]) / (1.0 - P_Sum);
}
else
{
    P = 1;
}
if (P > 1)
{
    P = 1;
}
G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
P_Sum = P_Sum + proportions2[kcount];
M = M - X[0];
if (X[0] > 0)
{
    NewV = Grid::GetTempWeed(ii, jj) + X[0];
    Grid::SetTempWeed(ii, jj, NewV);
    numSum = numSum + X[0];
}
}
delete[] state; //here we delete 'state'
state = NULL;
}
```

```

//Disperse the extra seeds in the direction of travel.
//Set the maximum value of j that the seeds can be dispersed to

int myrandd = rand() % maxd;
int myrandj = jcount + myrandd;
if (myrandj > NCols-1)
{
    myrandj = NCols-1;
}
else if (myrandj<0)
{
    myrandj = 0;
}

int extraseeds = numseeds - numSum;
int mynewS = Grid::GetTempWeed(icount, myrandj) + extraseeds;
Grid::SetTempWeed(icount, myrandj, mynewS);

}
}

void cultmoveW(std::vector<double> proportions2, int numseeds, int icount, int
    jcount, int maxd)
//move seeds by cultivation - cultivator moving west
{
    if (numseeds == 0) //if there are no seeds don't worry
    {
        return;
    }
    else
    {
        double P_Sum = 0; // to keep track of probability used so that we readjust
        int numSum = 0;
        int NRows = Grid::GetNumRows();
        int NCols = Grid::GetNumCols();
        int Len = proportions2.size();
        double NewV(0);
        int N = 1;
        int M = numseeds;
        for (int kcount = 0; kcount < Len; kcount++)
        {

            //The probability of landing in cell irow, jcol
            double P = proportions2[kcount];
            //
            *****
            ***** //
            //This sets up the nag functions to calculate the binomial outcome from
            numseeds events and P prob
            int const LR = 1;
            double R[LR];
            int X[1];

```

```

int ifail = 1;
int MODE = 3;
int const genid(1);
int const subid(0);
int lstate(17);
int* state; //when we declare 'state' we dont say how long it will be ↗
           so we need to delete it after we have used it
state = new int[lstate];
ifail = 1;
G05KGF(genid, subid, state, lstate, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05KGF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
if (kcount == 0) // For the first value in the array the seeds will be ↗
                dispersed into the starting square
{
    G05TAF(MODE, N, M, P, R, LR, state, X, ifail); //The number of ↗
           seeds that fall is X

    if (ifail != 0)
    {
        char myText[10];
        _itoa_s(ifail, myText, 10);
        char myBigText[50] = " Error in Nag G05TAF ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
    //
    //***** ↗
    //***** //
    P_Sum = P_Sum + proportions2[kcount];
    M = M - X[0];
    //Add into temporary weed structure
    NewV = Grid::GetTempWeed(icount, jcount) + X[0]; //The weeds that ↗
           were in centre cell + new dropped seeds
    Grid::SetTempWeed(icount, jcount, NewV);
    numSum = numSum + X[0]; //number of seeds that have dropped so far
}
else if (kcount > 0 && kcount <= 4)//For values of kcount from 1-4 ↗
           seeds will be dispersed in the opposite direction to the direction of↗
           travel
{
    int ii = icount;
    if (ii < 0)
    {
        ii = 0;
    }
    if (ii > NRows - 1)
    {
        ii = NRows - 1;
    }
}

```

```
int jj = jcount + kcount;
if (jj < 0)
{
    jj = 0;
}
if (jj > NCols - 1)
{
    jj = NCols - 1;
}

if (P < 1)
{
    P = (proportions2[kcount]) / (1 - P_Sum);
}
else
{
    P = 1;
}
if (P > 1)
{
    P = 1;
}

G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
if (ifail != 0)
{
    char myText[10];
    _itoa_s(ifail, myText, 10);
    char myBigText[50] = " Error in Nag G05TAF ";
    strcat_s(myBigText, myText);
    throw std::logic_error(myBigText);
}
P_Sum = P_Sum + proportions2[kcount];
M = M - X[0];
if (X[0] > 0)
{
    NewV = Grid::GetTempWeed(ii, jj) + X[0];
    Grid::SetTempWeed(ii, jj, NewV);
    numSum = numSum + X[0];
}
}
else //For values of k >4 seeds will be dispersed in the direction of ↗
travel
{
    int ii = icount;
    if (ii < 0)
    {
        ii = 0;
    }
    if (ii > NRows - 1)
    {
        ii = NRows - 1;
    }
    int jj = jcount - (kcount-4);
    if (jj < 0)
```

```

        {
            jj = 0;
        }
        if (jj>NCols - 1)
        {
            jj = NCols - 1;
        }

        if (P_Sum < 1)
        {
            P = (proportions2[kcount]) / (1 - P_Sum);
        }
        else
        {
            P = 1;
        }
        if (P>1)
        {
            P = 1;
        }
        G05TAF(MODE, N, M, P, R, LR, state, X, ifail);
        if (ifail != 0)
        {
            char myText[10];
            _itoa_s(ifail, myText, 10);
            char myBigText[50] = " Error in Nag G05TAF ";
            strcat_s(myBigText, myText);
            throw std::logic_error(myBigText);
        }
        P_Sum = P_Sum + proportions2[kcount];
        M = M - X[0];
        if (X[0] > 0)
        {
            NewV = Grid::GetTempWeed(ii, jj) + X[0];
            Grid::SetTempWeed(ii, jj, NewV);
            numSum = numSum + X[0];
        }
    }
    delete[] state;

}
//Disperse the extra seeds in the direction of travel.
//Set the maximum value of j that the seeds can be dispersed to

int myrandd = rand() % maxd;
int myrandj = jcount - myrandd;
if (myrandj > NCols-1)
{
    myrandj = NCols - 1;
}
else if (myrandj<0)
{
    myrandj = 0;
}

int extraseeds = numseeds-numSum;

```

---

```
    int mynewS = Grid::GetTempWeed(icount, myrandj) + extraseeds;  
    Grid::SetTempWeed(icount, myrandj, mynewS);  
  }  
}
```

```
#include "Water.h"
#include "math.h"
#include "LandGrid.h"
#include "weather.h"
#include <algorithm>

//std::ofstream ofm(Npath_buffer, std::ofstream::out | std::ofstream::app);

double hydrothermaltime(int irow, int jcol, double mya, int cultivationday) // ↗
    hydrothermal time is a function that uses weather data to determine the maximum ↗
    level of germination
{
    double gmd = 297.5; //%number of days from germination to maturity of mother ↗
        plants
    double wd = Grid::GetWD(irow,jcol); //%water deficit(mm) between flowering and↗
        maturity
    double depth = 1.5; //% depth of seed in cm
    double dh = 425; //%hydrothermal time spent in darkness before tillage
    double myph = Grid::GetPH(irow, jcol);

    double sw = 0.0014; //%mean seed weight(g)
    double n = 25; //%total available n(kg / ha)

    int maxdays = 50; //This is the maximum time period over which germination can ↗
        take place

        //table3 %Effect of seed characteristics and environmental ↗
        conditions of the proportion of non - dormant seeds, obtained ↗
        by selecting one equation from each section depending on ↗
        conditions and applying the five resulting equations in ↗
        sequence
        //i Loss of primary dormancy / after - ripening Effect of ↗
        seed characteristics
    double gm = 0.924 - 0.000149*gmd + 0.391*exp(-0.033*mya) - 0.00380*gmd*exp ↗
        (-0.033*mya) + 0.000777*wd;
    //Colbach and Durr(2003)

    // ii Effect of seed depth
    double gm1 = gm*(0.5311 - 0.00947*depth) / 0.5311;

    //iii Effect of stimulation by light while imbibed(during tillage or on soil ↗
        surface)
    double gm2 = gm1*exp(-0.00115*pow(dh, 1.121)); //Seeds activated during ↗
        current tillage
    // %Colbach et al 2002a)

    // % iv Effect of soil climate
    double gm3 = gm2;
    //Colbach et al 2002b)

    // % v Secondary dormancy due to winter conditions
    double gm4 = gm3;
    //Based on Lonchamp et al. (1984)

    // % table4 Effect of seed characteristics and environmental conditions of the↗
        germination parameters
```

```

// %i Loss of primary dormancy / after - ripening Effect of seed
characteristics(Colbach and Durr, 2003)
double gx0 = 49.78 - 66.43*exp(-0.0086*mya) - 0.0022*gmd + 0.358*gmd*exp
(-0.0086*mya); %%Germination lag
double gx50 = 65.72 + 200.99*exp(-0.044*mya) + 0.0968*gmd - 1.086*wd; %%Time
to mid - germination
double gb = 0.125 - 1.997*exp(-0.063*mya) + 0.00676*gmd + 0.0199*gmd*exp
(-0.063*mya) + 0.0101*wd + 246.9*sw - 0.00702*n; %%Shape parameter

// %ii Effect of seed depth
(extrapolated from experiment in this paper)
double varm = (0.5311 - 0.00947*depth) / 0.5311; %%Relative variation in the
proportion of non - dormant seeds
double gx01 = (1 / varm)*gx0; %%Germination lag
double gx501 = (1 / varm)*gx50; %%Time to mid - germination
double gb1 = (1 / varm)*gb; %%Shape parameter

// %iii Effect of stimulation by light while imbibed(during tillage or on soil
surface)
// % (Colbach et al., 2002a)
// % Seeds activated during current tillage
double gx02 = gx01;
double gx502 = gx501*(exp(0.212*pow(dh, 0.276)) - 1);
double gb2 = gb1;

%%iv = Effect of soil climate
double gx03 = gx02;
double gx503 = gx502;
double gb3 = gb2;

%%v Secondary dormancy due to winter conditions(extrapolated from Lonchamp et
al., 1984) Winter:
%%after Oct 20
int oct20 = 293; %%day number for october 20
int d = cultivationday + maxdays; %%day number for start of germination
double varm2 = (1 / 0.9481)*(-0.00317*(d - oct20) + 0.9481);
double gx04 = (1 / varm2)*gx03;
double gx504 = (1 / varm2)*gx503;
double gb4 = varm2*gb3;

if (gx04 < 0)
    gx04 = 0;
if (gb4 < 0.000001)
    gb4 = 0.000001;

double k = log(2); %%rate of increase
double a = gx04; %%lag phase
double c = gb4; %%shape parameter
double M = gm4;
double x50 = gx504;

if (myph < 6.5)
{
    M = M*40.92 / 36.72; %%values for low and high pH (asymptote is C parameter

```

```

    in gompertz curve - life cycle chapter)

}
double Germ(0);

//the function needs to access the soil information
double myClay = Grid::GetClay(irow, jcol);
double mySilt = Grid::GetSilt(irow, jcol);
double myOM = Grid::GetOC(irow, jcol);

double myElev = Grid::GetElevation(irow, jcol);
double myDb = Grid::GetBulkD(irow, jcol);
double mySoilDepth = Grid::GetSoilDepth(irow, jcol);
double myLat = Grid::GetLatitude(irow, jcol);

double myCell = Grid::GetCell();

double myWater = Grid::GetSWC(irow, jcol); //water saved in grid is for      ↗
    cultivationday

//// Set germination properties for black - grass

double WPb = -1.53; //Effect of environmental conditions on Alopecurus      ↗
    myosuroides germination.II.Effect of moisture conditions and storage length.N↗
    COLBACH*, C DU` RR, B CHAUVEL* & G RICHARD.European Weed Research Society  ↗
    Weed Research 2002 42, 222-230.

double Tb = 0; //Effect of environmental conditions on Alopecurus myosuroides ↗
    germination.I.Effect of temperature and light.N COLBACH*, B CHAUVEL*, C DU` ↗
    RR & G RICHARD.European Weed Research Society Weed Research 2002 42, 210-221

////Accumulate hydrothermal time
double mylength = maxdays + 1;
double TT(0);
double WhTT(0);
double HTT = 0;

for (int i = 0; i < mylength; i++) // for each day after cultivation
{

    int iDay = i + cultivationday - 1;
    //get that days weather data

    double Irr = Weath::GetIrrad(0, iDay);
    double EMVP = Weath::GetVapP(0, iDay);
    double AvRad = Irr * 1000;
    double Vap = EMVP * 10;

    TT = TT + Weath::GetTT(0, iDay); //add the thermal time for htat day on to ↗
        the thermal time already accumulated

    // Calculte the hydrotime
    double Tmin = Weath::GetMinT(0, iDay);
    double Tmax = Weath::GetMaxT(0, iDay);

```

```
double Wind = Weath::GetWindS(0, iDay);
double E0 = 0;
double ES0 = 0;
double ET0 = 0;
Penman(iDay, irow, jcol, E0, ES0, ET0); //use the Penman function to calculate evapotranspiration based on soil and weather data. This function is in water.cpp
double myPrecip = Weath::GetPrecip(0, iDay);

double wc = myWater*mySoilDepth; //convert to mm
wc = wc + myPrecip - ES0; //adjust the soil water content according to the days precip and evapotranspiration
myWater = wc / mySoilDepth; //convert back to VWC
double myw50, myw15000;
double mbar = 50;
vanGenuchten2(irow, jcol, mbar, myw50); //calculate water content needed for mbar=50 (field capacity)
mbar = 15000;
vanGenuchten2(irow, jcol, mbar, myw15000); //calculate water content needed for mbar=15000 (wilting point)
if (myWater < myw15000) //prevents van genuchten from working correctly
{
    myWater = myw15000;
}
if (myWater > myw50) //prevents van genuchten from working correctly
{
    myWater = myw50;
}

mbar = vanGenuchten(irow, jcol, myWater);

////Convert mbar to MPa
double WP = mbar * -0.0001;

double ht = 0; //hydrotime
if (WP > WPb)
{
    ht = WP - WPb;
}
double tt = Weath::GetTT(0, iDay); //thermal time

double htt = tt*ht; //hydrothermal time
WhTT = WhTT + Weath::GetWhTT(0, iDay);

//Check the green area index of the wheat. Once the wheat is sufficiently big, black-grass germination will cease
double GAI = StorkeyGAI(WhTT, myCell); //StorkeyGAI is a function to calculate GAI of wheat it is in Water.cpp
if (GAI <= 0.5) //if the wheat is sufficiently small
{
    HTT = HTT + htt; //add that days hydrothermal time on to the hydrothermal time accumulated so far
}
```

```
    if (HTT < a + 49.169) //if we are still in the lag phase of germination
    {
        Germ = 0;
    }
    else//after the lag phase we have an exponential phase
    {
        double DivBit = (HTT - a - 49.169) / (x50 - a);

        Germ = M*(1 - pow(exp(-k*(DivBit)), c));
    }

}

return Germ;

}

void initialwater(double irow, double jcol, double& myWater, double startday,
double endday)
//This is a function to initialise the soil water content from the start day to end
day
{
    for (int iday = startday; iday < endday; iday++) //for each day calculate the
water gained and lost according to weather conditions
    {
        //Interrogate the weather data - these functions read the weather data and
are in Weather.cpp
        double Irr, EMVP, Precip, AvRad, Vap;
        Irr = Weath::GetIrrad(0, iday);
        EMVP = Weath::GetVapP(0, iday);
        Precip = Weath::GetPrecip(0, iday);
        AvRad = Irr * 1000;
        Vap = EMVP * 10;

        double myDepth = Grid::GetSoilDepth(irow, jcol);
        double E0 = 0;
        double ES0 = 0;
        double ET0 = 0;
        Penman(iday, irow, jcol, E0, ES0, ET0); //calculate evaporation from the
soil using Penman function in Water.cpp

        double wc = myWater*myDepth; //convert to mm
        wc = wc + Precip - ES0; //adjust the soil water content according to the
days precip and evapotranspiration
        myWater = wc / myDepth; //convert back to VWC]

        double myw50, myw15000;
        double mbar = 50;
        vanGenuchten2(irow, jcol, mbar, myw50); //calculate water content needed
for mbar=50
        mbar = 15000;
        vanGenuchten2(irow, jcol, mbar, myw15000); //calculate water content needed
for mbar=15000
        if (myWater <= myw15000) //prevents van genuchten from working correctly
        {
```

```

        myWater = myw15000;
    }
    if (myWater >= myw50) //prevents van genuchten from working correctly
    {
        myWater = myw50;
    }
}
}

void waterdeficit(double irow, double jcol, double& myWater, double startday,
double endday, double& mydeficit)
//This is a function to calculate the water deficit between flowering and harvest
in the previous season
{
    for (int iday = startday; iday < endday; iday++) //for each day calculate
        the water gained and lost according to weather conditions
    {
        //Interrogate the weather data - these functions read the weather data and
        are in Weather.cpp
        double Irr, EMVP, Precip, AvRad, Vap;
        Irr = Weath::GetIrrad(0, iday);
        EMVP = Weath::GetVapP(0, iday);
        Precip = Weath::GetPrecip(0, iday);
        AvRad = Irr * 1000;
        Vap = EMVP * 10;

        double myDepth = Grid::GetSoilDepth(irow, jcol);
        double E0 = 0;
        double ES0 = 0;
        double ET0 = 0;
        Penman(iday, irow, jcol, E0, ES0, ET0); //calculate evaporation from the
        soil using Penman function in Water.cpp
        double wc = myWater*myDepth; //convert to mm

        if (ET0>(Precip + wc))
            mydeficit = mydeficit + (ET0 - (Precip + wc)); //calculate the deficit
        wc = wc + Precip - ES0; //adjust the soil water content according to the
        days precip and evapotranspiration
        myWater = wc / myDepth; //convert back to VWC

        double myw50, myw15000;
        double mbar = 50;
        vanGenuchten2(irow, jcol, mbar, myw50); //calculate water content needed
        for mbar=50
        mbar = 15000;
        vanGenuchten2(irow, jcol, mbar, myw15000); //calculate water content needed
        for mbar=15000
        if (myWater <= myw15000) //prevents van genuchten from working correctly
        {
            myWater = myw15000;
        }
        if (myWater >= myw50) //prevents van genuchten from working correctly
        {

```

```
        myWater = myw50;
    }

}

}

void resetwater(double irow, double jcol)//no longer needed
//This is a function to initialise the soil water content based on the weather data ↗
in the previous year
{
    double myWater = Grid::GetSWC(irow, jcol);

    double startday = 76;//This is the Julian day for which the soil water content ↗
is valid - so the day the field measurements were taken
        //CrossF = 21
        //Redb = 71
        //Iv = 85
        //Hav 76

    for (int myi = startday; myi < 365 + startday; myi++) //for each day up until ↗
the day of ploughing calculate the water gained and lost according to weather ↗
conditions
    {
        int iday;
        if (myi < 365)
        {
            iday = myi;
        }
        else
        {
            iday = myi - 365;
        }
        //Interrogate the weather data - these functions read the weather data and ↗
are in Weather.cpp
        double Irr, EMVP, Precip, AvRad, Vap;
        Irr = Weath::GetIrrad(0, iday);
        EMVP = Weath::GetVapP(0, iday);
        Precip = Weath::GetPrecip(0, iday);
        AvRad = Irr * 1000;
        Vap = EMVP * 10;

        double myDepth = Grid::GetSoilDepth(irow, jcol);
        double E0 = 0;
        double ES0 = 0;
        double ET0 = 0;
        Penman(iday, irow, jcol, E0, ES0, ET0); //calculate evaporation from the ↗
soil using Penman function in Water.cpp
        double wc = myWater*myDepth; //convert to mm
        wc = wc + Precip - ES0; //adjust the soil water content according to the ↗
days precip and evapotranspiration
        myWater = wc / myDepth; //convert back to VWC

        double myw50, myw15000;
        double mbar = 50;
        vanGenuchten2(irow, jcol, mbar, myw50); //calculate water content needed ↗
```

```

        for mbar=50
        mbar = 15000;
        vanGenuchten2(irow, jcol, mbar, myw15000); //calculate water content needed
        for mbar=1500
        if (myWater <= myw15000) //prevents van genuchten from working correctly
        {
            myWater = myw15000;
        }
        if (myWater >= myw50) //prevents van genuchten from working correctly
        {
            myWater = myw50;
        }
    }
    Grid::SetSWC(irow, jcol, myWater);
}

```

```

double StorkeyGAI(double TT, double myCell)
//StorkeyGAI is a function that calculates the green area index of the wheat plants
based on accumulated thermal time
//From Storkey&Cussans 2000
{
    double Cm = 0.32;//5.8; //max relative growth rate
    double RGRm = 0.00575;//0.3; //max growth rate
    double t0 = 630; //degreedays time at which plant reaches linear phase of
growth
    double W = (Cm / RGRm)*log(1 + exp(RGRm*(TT - t0)));

    double Wm = W / 10000;
    double cellA = myCell*myCell;
    double wheat = 300 * cellA;
    double GA = (Wm*wheat);
    double GAI = GA / cellA;

    return GAI;
}

```

```

void Penman(int iDay, int irow, int jcol, double& E0, double& ES0, double& ET0)
/*Penman function for calculating evapotranspiration
This calculates the potential evapotranspiration rates from a free water
surface(E0), a bare soil surface(ES0), and a crop canopy(ET0) in mm / d.
For these calculations the analysis by Penman is followed(Frere and
Popov, 1979; Penman, 1948, 1956, and 1963).*/
{
    //Declare Parameters
    double PsyCon, RefCFW, RefCFS, RefCFC, LHVAP, STBC, AngstA, AngstB, MinR, MaxR;
    PsyCon = 0.67; //psychrometric instrument constant(mbar / Celsius - 1)
    RefCFW = 0.05; //albedo for water surface
    RefCFS = 0.15; //albedo for soil surface
    RefCFC = 0.25; //albedo for canopy
    LHVAP = 2.45E6; //latent heat of evaporation of water(J / kg = J / mm)
    STBC = 4.9E-3; // Stefan Boltzmann constant(J / m2 / d / K4)
}

```

```

AngstA = 0.25; // Empirical constants in Angstrom formula -
AngstB = 0.50; // FAO recommend 0.25 and 0.50
MinR = 0.0;
MaxR = 1.0;

// Preparatory calculations
// *   mean daily temperature and temperature difference(Celsius)
// *   coefficient Bu in wind function, dependent on temperature
// *   difference
double Tmin, Tmax, AvTemp, Tdif, Irr, AvRad, x, BU, Pbar, myElev, gamma, A;
Tmin = Weath::GetMinT(0, iDay);
Tmax = Weath::GetMaxT(0, iDay);
AvTemp = (Tmin + Tmax) / 2.0; //mean daily temperature
Tdif = Tmax - Tmin; //temperature difference
double pardif, paddir, myscale;
splitirrad(iDay, irow, jcol, pardif, paddir);
myscale = Grid::GetSolarScale(irow, jcol);
AvRad = pardif + (paddir*myscale);
myElev = Grid::GetElevation(irow, jcol);

x = (Tdif - 12.0) / 4.0;
double myLimit = mylimitfn(MinR, MaxR, x);

BU = 0.54 + 0.35*myLimit; //coefficient Bu in wind function is dependent on  ↗
    temperature difference

Pbar = 1013.0*exp(-0.034*myElev / (AvTemp + 273.0)); //barometric pressure  ↗
    (mbar)
gamma = PsyCon*Pbar / 1013.0; //psychrometric constant(mbar / Celsius)

/*saturated vapour pressure
saturated vapour pressure according to equation of Goudriaan
(1977) derivative of SVAP with respect to temperature, i.e.
slope of the SVAP - temperature curve(mbar / Celsius);
measured vapour pressure not to exceed saturated vapour pressure*/

double SVap, delta, EMVP, Vap;
EMVP = Weath::GetVapP(0, iDay);
Vap = EMVP * 10;
SVap = 6.10588*exp(17.32491*AvTemp / (AvTemp + 238.102));
delta = 238.102*17.32491*SVap / pow((AvTemp + 238.102), 2);
Vap = fmin(Vap, SVap);

/*RELSSD
the expression n / N(RELSSD) from the Penman formula is estimated
from the Angstrom formula : RI = RA(A + B.n / N)->n / N = (RI / RA - A) / B,
where RI / RA is the atmospheric transmission obtained by the astro
function*/

double ATMTR, amax, mymax, RELSSD;
ATMTR = astro(irow, jcol, iDay);
amax = (ATMTR - abs(AngstA)) / abs(AngstB);
mymax = fmax(0, amax);
RELSSD = fmin(1, mymax);

/*Terms in Penman formula, for water, soil and canopy

```

```

net outgoing long - wave radiation(J / m2 / d) acc.to Brunt(1932)*/

double RB, RNW, RNS, RNC;

RB = STBC*pow((AvTemp + 273), 4)*(0.56 - 0.079*sqrt(Vap))*(0.1 + 0.9*RELSSD);
// net absorbed radiation, expressed in mm / d
RNW = (AvRad*(1 - RefCFW) - RB) / LHVAP;
RNS = (AvRad*(1 - RefCFS) - RB) / LHVAP;
RNC = (AvRad*(1 - RefCFC) - RB) / LHVAP;

// evaporative demand of the atmosphere(mm / d)
double EA, EAC, Wind;
Wind = Weath::GetWindS(0, iDay);
amax = (SVap - Vap);
mymax = fmax(0, amax);
EA = 0.26*mymax*(0.5 + BU*Wind);
EAC = 0.26*mymax*(1.0 + BU*Wind);

// Penman formula(1948)
E0 = (delta*RNW + gamma*EA) / (delta + gamma);
ES0 = (delta*RNS + gamma*EA) / (delta + gamma);
ET0 = (delta*RNC + gamma*EAC) / (delta + gamma);

//Ensure reference evaporation >= 0.
E0 = fmax(0, E0);
ES0 = fmax(0, ES0);
ET0 = fmax(0, ET0);

}

double mylimitfn(double MinR, double MaxR, double x)//used in Penman
{
double myLimit;
if (x < MinR)
{
myLimit = MinR;
}
else if (x <= MaxR)
{
myLimit = x;
}
else
{
myLimit = MaxR;
}

return myLimit;
}

double astro(int irow, int jcol, int iDay)
{
/* Astro function for calculating astronomical values
% astronomic daylength, diurnal radiation characteristics such as the
% atmospheric transmission, diffuse radiation etc.
% This routine has been modified so that it uses arrays to hold some input

```

```

% output variables for faster processing */

//Declare Parameters
double Angle, Rad, Dec, SC, pi;
pi = atan(1) * 4;
Angle = -4.0;
Rad = 0.0174533;
Dec = -asin(sin(23.45*Rad)*cos(2 * pi*(iDay + 10.0) / 365.0)); //Declination
SC = 1370.0*(1.0 + 0.033*cos(2 * pi*iDay / 365.0)); //solar constant

// Calculation of daylength from intermediate variables
double Lat, SinLD, CosLD, AOB;
Lat = Grid::GetLatitude(irow, jcol);
SinLD = sin(Rad*Lat)*sin(Dec);
CosLD = cos(Rad*Lat)*cos(Dec);
AOB = SinLD / CosLD;

/* Winter Limit
For very high latitudes and days in summer and winter a limit is
inserted to avoid math errors when daylength reaches 24 hours in
summer or 0 hours in winter.*/

//Calculate solution for base = 0 degrees
double DayL, DsinB, DsinBE;

if (abs(AOB) <= 1)
{
    DayL = 12 * (1 + 2 * asin(AOB) / pi);
    DsinB = 3600 * (DayL*SinLD + 24 * CosLD*sqrt(1 - pow(AOB, 2)) / pi);
    DsinBE = 3600.*(DayL*(SinLD + 0.4*(pow(SinLD, 2) + pow(CosLD, 2)*0.5)) + 12 *
        * CosLD*(2 + 3 * 0.4*SinLD)*sqrt(1 - pow(AOB, 2)) / pi);
}
else if (AOB > 1)
{
    DayL = 24;
    DsinB = 3600 * (DayL*SinLD);
    DsinBE = 3600 * (DayL*(SinLD + 0.4*(pow(SinLD, 2) + pow(CosLD, 2)*0.5)));
}
else if (AOB < -1)
{
    DayL = 0;
    DsinB = 3600 * (DayL*SinLD);
    DsinBE = 3600 * (DayL*(SinLD + 0.4*(pow(SinLD, 2) + pow(CosLD, 2)*0.5)));
}

//Calculate solution for base = -4 degrees
double AOBcorr, DayLP;
AOBcorr = (-sin(Angle*Rad) + SinLD) / CosLD;
if (abs(AOBcorr) <= 1)
{
    DayLP = 12.*(1 + 2.*asin(AOBcorr) / pi);
}
else if (AOBcorr > 1)
{
    DayLP = 24;
}

```

```
}
else if (AOBcorr < -1)
{
    DayLP = 0;
}

// extraterrestrial radiation and atmospheric transmission
double angot, ATMTR;
angot = SC*DsinB;
// Check for DayL = 0 as in that case the angot radiation is 0 as well
double Irr, AvRad;
Irr = Weath::GetIrrad(0, iDay);
AvRad = Irr * 1000;

if (DayL>0)
{
    ATMTR = AvRad / angot;
}

else
{
    ATMTR = 0;
}

// estimate fraction diffuse irradiation
double FRDIF, DifPP;

if (ATMTR > 0.75)
{
    FRDIF = 0.23;
}
else if (ATMTR <= 0.75 & ATMTR > 0.35)
{
    FRDIF = 1.33 - 1.46*ATMTR;
}
else if (ATMTR <= 0.35 & ATMTR > 0.07)
{
    FRDIF = 1 - 2.3*pow((ATMTR - 0.07), 2);
}
else if (ATMTR <= 0.07)
{
    FRDIF = 1;
}

DifPP = FRDIF*ATMTR*0.5*SC;

return ATMTR;
}

double vanGenuchten(int irow, int jcol, double myWater)
{
    /*vanGenuchten is a pedotransfer function that uses known soil properties
    to calculate the water potential*/

    //Calculate parameters for equations
    double myClay, mySilt, myOM, myDb, alpha, thetaS, n, thetaR, m;
```

```

myClay = Grid::GetClay(irow, jcol) / 100;
mySilt = Grid::GetSilt(irow, jcol) / 100;
myOM = Grid::GetOC(irow, jcol);
myDb = Grid::GetBulkD(irow, jcol);

alpha = exp(-14.96 + 3.135*myClay + 3.51*mySilt + 0.646*(myOM*1.72) +
15.29*myDb
- 0.192 * 1 - 4.671*pow(myDb, 2) - 7.81*pow(myClay, 2) - 0.00687*pow
((myOM*1.72), 2)
+ 0.0449*pow((myOM*1.72), -1) + 0.0663*log(mySilt * 100) + 0.1482*log
(myOM*1.72)
- 4.546*myDb*mySilt - 0.4852*myDb*(myOM*1.72) + 0.673*myClay * 1);

thetaS = 0.7919 + 0.1691*myClay - 0.29619*myDb - 0.01491*pow(mySilt, 2)
+ 0.0000821*pow((myOM*1.72), 2) + 0.02427*pow((myClay * 100), -1) +
0.01113*pow((100 * mySilt), -1)
+ 0.01472*log(mySilt * 100) - 0.00733*(myOM*1.72)*myClay -
0.0619*myDb*myClay
- 0.001183*myDb*(myOM*1.72) - 0.01664*mySilt * 1;

n = exp(-25.23 - 2.195*myClay + 0.74*mySilt - 0.194*(myOM*1.72) + 45.5*myDb -
7.24*pow(myDb, 2)
+ 3.658*pow(myClay, 2) + 0.002885*pow((myOM*1.72), 2) - 12.81*pow(myDb, -1)
- 0.1524*pow((100 * mySilt), -1) - 0.01958*pow((myOM*1.72), -1) -
0.2876*log(mySilt * 100)
- 0.0709*log(myOM*1.72) - 44.6*log(myDb) - 2.264*myDb*myClay + 0.0896*myDb*
(myOM*1.72)
+ 0.718*myClay * 1) + 1;

thetaR = 0.01;

m = 1 - 1 / n;

// Convert water content in soil(%) to water potential
double mbar, top, bottom, power1, part1, power2, part2;
top = thetaR - thetaS;
bottom = thetaR - myWater;
power1 = 1 / m;
part1 = pow((top / bottom), power1);
power2 = 1 / n;
part2 = pow((part1 - 1), power2);
mbar = part2 / alpha;

return mbar;
}

double vanGenuchten2(int irow, int jcol, double mbar, double& myWater)
{

//vanGenuchten is a pedotransfer function that uses known soil properties
to calculate the water percentage*/

//Calculate parameters for equations
double myClay, mySilt, myOC, myDb, alpha, thetaS, n, thetaR, m;
myClay = Grid::GetClay(irow, jcol) / 100; // convert clay to proportions

```

```

mySilt = Grid::GetSilt(irow, jcol) / 100; // convert silt to proportions
myOC = Grid::GetOC(irow, jcol); // Organic carbon is transform to organic
matter by multiplying by 1.72 below
myDb = Grid::GetBulkD(irow, jcol);

alpha = exp(-14.96 + 3.135*myClay + 3.51*mySilt + 0.646*(myOC*1.72) +
15.29*myDb - 0.192 * 1 - 4.671*pow(myDb, 2)
- 7.81*pow(myClay, 2) - 0.00687*pow((myOC*1.72), 2) + 0.0449*pow
((myOC*1.72), -1) + 0.0663*log(mySilt * 100)
+ 0.1482*log(myOC*1.72) - 4.546*myDb*mySilt - 0.4852*myDb*(myOC*1.72) +
0.673*myClay * 1);

thetaS = 0.7919 + 0.1691*myClay - 0.29619*myDb - 0.01491*pow(mySilt, 2) +
0.0000821*pow((myOC*1.72), 2)
+ 0.02427*pow((myClay * 100), -1) + 0.01113*pow((100 * mySilt), -1) +
0.01472*log(mySilt * 100)
- 0.00733*(myOC*1.72)*myClay - 0.0619*myDb*myClay - 0.001183*myDb*
(myOC*1.72) - 0.01664*mySilt * 1;

n = exp(-25.23 - 2.195*myClay + 0.74*mySilt - 0.194*(myOC*1.72) + 45.5*myDb -
7.24*pow(myDb, 2)
+ 3.658*pow(myClay, 2) + 0.002885*pow((myOC*1.72), 2) - 12.81*pow(myDb, -1)
- 0.1524*pow((100 * mySilt), -1)
- 0.01958*pow((myOC*1.72), -1) - 0.2876*log(mySilt * 100) - 0.0709*log
(myOC*1.72) - 44.6*log(myDb)
- 2.264*myDb*myClay + 0.0896*myDb*(myOC*1.72) + 0.718*myClay * 1) + 1;

thetaR = 0.01;

m = 1 - 1 / n;

// Convert waterpotential in soil to water content(%)
myWater = (thetaR + (thetaS - thetaR) / pow(1 + pow((alpha*mbar), n), m));

return myWater;
}

void averageWVC(double irow, double jcol, double& myWater, double startday, double
endday, double& sumWVC, int& countdays)//This is a function to initialise the
soil water content based on the weather data in the previous year
{
for (int iday = startday; iday < endday; iday++) //for each day calculate the
water gained and lost according to weather conditions
{
//Interrogate the weather data - these functions read the weather data and
are in Weather.cpp
double Irr, EMVP, Precip, AvRad, Vap;
Irr = Weath::GetIrrad(0, iday);
EMVP = Weath::GetVapP(0, iday);
Precip = Weath::GetPrecip(0, iday);
AvRad = Irr * 1000;
Vap = EMVP * 10;

double myDepth = Grid::GetSoilDepth(irow, jcol);
double E0 = 0;

```

```

double ES0 = 0;
double ET0 = 0;
Penman(iday, irow, jcol, E0, ES0, ET0); //calculate evaporation from the soil using Penman function in Water.cpp ↗

double wc = myWater*myDepth; //convert to mm
wc = wc + Precip - ES0; //adjust the soil water content according to the days precip and evapotranspiration ↗
myWater = wc / myDepth; //convert back to VWC]

double myw50, myw15000;
double mbar = 50;
vanGenuchten2(irow, jcol, mbar, myw50); //calculate water content needed for mbar=50 ↗
mbar = 15000;
vanGenuchten2(irow, jcol, mbar, myw15000); //calculate water content needed for mbar=15000 ↗
if (myWater <= myw15000) //prevents van genuchten from working correctly
{
    myWater = myw15000;
}
if (myWater >= myw50) //prevents van genuchten from working correctly
{
    myWater = myw50;
}

sumVWC = sumVWC + myWater;
countdays = countdays + 1;
}
}

double solarenergy(double Latitude, double Slope, double Aspect)//calculates the solar energy for a given latitude, slope and aspect ↗
{
    // Based on equations given by E.C.Frank and R.Lee(1966)
    // U.S. Forestry service research paper RM - 18.

    double klat = 1;//assume latitude is constant for the wohole field
    double DEC[13] = { 0.4102, 0.3834, 0.3374, 0.2717, 0.1905, 0.0983, 0.0, ↗
        -0.0983, -0.1905, -0.2717, -0.3374, -0.3834, -0.4102 };
    double NDAYS[13] = { 21, 34, 29, 29, 29, 29, 29, 29, 28, 28, 32, 19 };
    double IOE[13] = { 1.347, 1.350, 1.355, 1.362, 1.371, 1.382, 1.392, 1.404, ↗
        1.414, 1.423, 1.430, 1.436, 1.438 }; // **** SOLAR CONSTANT ASSUMED AS 1.39 ↗
        KW / M**2
    double LAT = Latitude*0.01745;
    double GRAD = Slope*0.01745;
    double AZI = Aspect*0.01745;
    if (LAT>1.5696)
    {
        LAT = 1.5696;
    }

    //*** COMPUTE TIMES OF SUNRISE AND SUNSET FOR SOLAR DECLINATIONS
    double sunris[13];
    double sunset[13];

```

```

for (int jcount = 1; jcount < 14; jcount++)
{
    double DELTA = DEC[jcount];
    double WTCOS = -(sin(LAT) / cos(LAT))*(sin(DELTA) / cos(DELTA));
    if (abs(WTCOS)<1.0E-10)
        WTCOS = 1.0E-10;
    if (WTCOS > 0.9999)
    {
        sunris[jcount-1] = 0.0;
        sunset[jcount - 1] = 0.0;
    }
    else if (WTCOS < -0.9999)
    {
        sunris[jcount - 1] = -12.0;
        sunset[jcount - 1] = 12.0;
    }
    else
    {
        double WTTAN = abs(sqrt(1.0 - WTCOS*WTCOS) / WTCOS);
        double WT = atan(WTTAN);
        if (WTCOS<0.0)
            WT = 3.14159 - WT;
        sunris[jcount - 1] = -WT*3.819;
        sunset[jcount - 1] = WT*3.819;
    }
}

/** COMPUTE LATITUDE OF EQUIVALENT SLOPE, THETA, AND
// LONGITUDE SHIFT, ALPHA, FOR SITE
double THSIN = sin(GRAD)*cos(AZI)*cos(LAT) + cos(GRAD)*sin(LAT);
if (THSIN>0.99999)
    THSIN = 0.99999;
if (THSIN<-0.99999)
    THSIN = -0.99999;
double THTAN = THSIN / sqrt(1.0 - THSIN*THSIN);
double THETA = atan(THTAN);
double DIV = cos(GRAD)*cos(LAT) - cos(AZI)*sin(GRAD)*sin(LAT);
double ALTAN;
if (abs(DIV) >= 1.0E-10)
    ALTAN = sin(AZI)*sin(GRAD) / DIV;
else
    ALTAN = 1.0E10;
double ALPHA = atan(ALTAN);

/** CALCULATE SOLAR RADIATION FOR EACH DAY WITH GIVEN
// DECLINATION AND SUM
double ENERGY = 0.0;
for (int jcount = 1; jcount < 14; jcount++)
{
    double DELTA = DEC[jcount];
    double TCOSP = -(sin(THETA) / cos(THETA))*(sin(DELTA) / cos(DELTA));
    double T1, T2;
    if (abs(TCOSP)<1.0E-10)
        TCOSP = 1.0E-10;
    if (TCOSP > 0.9999)

```

```

    {
        T1 = 0.0;
        T2 = 0.0;
    }
    else if (TCOSP < -0.9999)
    {
        T1 = -12.0;
        T2 = 12.0;
    }
    else
    {
        double TTANP = abs(sqrt(1.0 - TCOSP*TCOSP) / TCOSP);
        double WTP = atan(TTANP);
        if (TCOSP < 0.0)
            WTP = 3.14159 - WTP;
        T1 = (-WTP - ALPHA)*3.819;
        T2 = (WTP - ALPHA)*3.819;
    }
    if (T1<sunris[jcount - 1])
        sunris[jcount - 1];
    if (T2>sunset[jcount - 1])
        T2 = sunset[jcount - 1];
    double SRAD = IOE[jcount - 1]*((T2 - T1)*sin(THETA)*sin(DELTA) + 3.819*cos ↗
        (THETA)*cos(DELTA)*(sin(0.2618*T2) - sin(0.2618*T1)))*3.6;
    ENERGY = ENERGY + SRAD*NDAYS[jcount - 1];
}
return ENERGY;
}

```

```

void refsolar()//Get reference value for solar energy and compute total potential ↗
energy for each cell in the field.
//Compare them to the reference to give a scaling factor for each cell dependent on ↗
slope and aspect
{

```

```

    double MyLat = Grid::GetLatitude(1, 1);
    double RefSolarE;
    RefSolarE = solarenergy(MyLat, 0, 0);//Get reference value for solar energy on ↗
a flat surfact

```

```

    double slope, aspect, energy, scalesolar;

```

```

    for (int irow = 0; irow < Grid::GetNumRows(); irow++)

```

```

    {
        for (int jcol = 0; jcol < Grid::GetNumCols(); jcol++)//For each cell in the ↗
field

```

```

    {
        slope = Grid::GetSlope(irow, jcol);
        aspect = Grid::GetAspect(irow, jcol);
        //compute total potential energy for each cell in the field.
        energy = solarenergy(MyLat, slope, aspect);
        //Compare them to the reference to give a scaling factor for each cell ↗
dependent on slope and aspect
        scalesolar = energy / RefSolarE;
        Grid::SetSolarScale(irow, jcol, scalesolar);
    }
}

```

```

    }
}

void splitirrad(int iday, int irow, int jcol, double& pardif, double& pardir)
//separate the incoming radiation into direct and diffuse components
{
    double Irr, AvRad, Lat, SinLD, CosLD;
    double pi = 3.1415926;
    Irr = Weath::GetIrrad(0, iday);
    Lat = Grid::GetLatitude(irow, jcol);
    AvRad = Irr * 1000;
    double Rad = 0.0174533;
    double Dec = -asin(sin(23.45*Rad)*cos(2 * pi*(iday + 10.0) / 365.0)); // ↗
    Declination
    SinLD = sin(Rad*Lat)*sin(Dec);
    CosLD = cos(Rad*Lat)*cos(Dec);

    double aob = SinLD / CosLD;
    double DayL = 12 * (1 + 2 * asin(aob) / pi);
    double hour = 20;
    double sinb = fmax(0, SinLD + CosLD*cos(2 * pi*(hour + 12) / 24)); //sine of ↗
    solar elevation
    double dsinb = 3600*(DayL*SinLD + 24 * CosLD*sqrt(1 - aob*aob) / pi); //integral ↗
    of sin b
    double dsinbe = 3600 * (DayL*(SinLD + 0.4*(SinLD*SinLD + CosLD*CosLD*0.5)) + ↗
    12.0*CosLD*(2.0+3.0*0.4*SinLD)*sqrt(1 - aob*aob) / pi); //integral of sinb ↗
    with correction for lower atmospheric transmission at low solar elevations

    double sc = 1370 * (1 + 0.033*cos(2*pi*iday/365)); //solar constant
    double angot = sc*dsinb; //daily extraterrestrial radiation

    double atmtr = AvRad / angot; //atmospheric transmission
    double frdif; //diffuse light fraction
    if (atmtr > 0.75)
        frdif = 0.23;
    if (atmtr <= 0.75 && atmtr > 0.35)
        frdif = 1.33 - 1.46*atmtr;
    if (atmtr <= 0.35 && atmtr > 0.07)
        frdif = 1 - 2.3*pow((atmtr - 0.07),2);
    if (atmtr <= 0.07)
        frdif = 1;

    pardif = AvRad*frdif;
    pardir = AvRad - pardif;
}

```

```
#include "Weather.h"
#include <fstream>

//This code is all to handle the Weather class
//By AE Milne
Weather::Weather()//constructor
{
    Firstyear=-1;
}
Weather::~Weather() //destructor
{
    irrad.clear(); //(kJ m-2 d-1)
    minTemp.clear();//(degrees Celsius)
    maxTemp.clear(); //(degrees Celsius)
    vapPres.clear(); //early morning vapour pressure (kPa)      Zeroes average ↗
    of surrounding days
    windSpeed.clear(); //speed (height: 2 m?) (m s-1)
    precip.clear(); //(mm d-1)
    sunHours.clear();
}

void Weather::AddIrrad(double myIrrad)
{
    irrad.push_back(myIrrad);
}

void Weather::AddMaxT(double myMaxT)
{
    maxTemp.push_back(myMaxT);
}

void Weather::AddMinT(double myMinT)
{
    minTemp.push_back(myMinT);
}

void Weather::AddVapP(double myVapP)
{
    vapPres.push_back(myVapP);
}

void Weather::AddWindS(double myWindS)
{
    windSpeed.push_back(myWindS);
}

void Weather::AddPrecip(double myprecip)
{
    precip.push_back(myprecip);
}

void Weather::AddsunHours(double mySun)
{
    sunHours.push_back(mySun);
}
```

```
void Weather::AddTT(double mytt)
{
    TT.push_back(mytt);
}
void Weather::AddWhTT(double myWhTT)
{
    WhTT.push_back(myWhTT);
}
void Weather::SetFirstYear(int myYear)
{
    Firstyear=myYear;
}
double Weather::GetIrrad(int iday)
{
    if (iday<irrad.size())
        return irrad[iday];
    else
    {
        char myText[10];
        _itoa_s(iday, myText, 10);
        char myBigText[50] = " index out of bounds in irrad array ";
        strcat_s(myBigText, myText);
        throw std::logic_error(myBigText);
    }
}

double Weather::GetMaxT(int iday)
{
    if (iday<maxTemp.size())
        return maxTemp[iday];
    else
        throw std::logic_error("index out of bounds in maxTemp array");
}

double Weather::GetMinT(int iday)
{
    if (iday<minTemp.size())
        return minTemp[iday];
    else
        throw std::logic_error("index out of bounds in minTemp array");
}

double Weather::GetVapP(int iday)
{
    if (iday<vapPres.size())
        return vapPres[iday];
    else
        throw std::logic_error("index out of bounds in vapPres array");
}

double Weather::GetWindS(int iday)
{

```

```
    if (iday<windSpeed.size())
        return windSpeed[iday];
    else
        throw std::logic_error("index out of bounds in windSpeed array");
}

double Weather::GetTT(int iday)
{
    if (iday<TT.size())
        return TT[iday];
    else
        throw std::logic_error("index out of bounds in TT array");
}

double Weather::GetWhTT(int iday)
{
    if (iday<WhTT.size())
        return WhTT[iday];
    else
        throw std::logic_error("index out of bounds in WhTT array");
}

double Weather::GetPrecip(int iday)
{
    if (iday<precip.size())
        return precip[iday];
    else
        throw std::logic_error("index out of bounds in precip array");
}

double Weather::GetsunHours(int iday)
{
    if (iday<sunHours.size())
        return sunHours[iday];
    else
        throw std::logic_error("index out of bounds in sunHours array");
}

int Weather::GetFirstYear()
{
    return Firstyear;
}

//This is the main namespace where the weather data will be held
namespace Weath
{
    Weather Weath0; //these are the objects that hold the weather.
    Weather Weath1;

    void ReadInWeath(int SetNum, char FName[], int iniYear)//reads in the weather data from a specified set of files into Weath'SetNum'
    {
        if ((SetNum!=0)&(SetNum!=1))
            throw std::logic_error("Weather set number not valid");
        //open weather one file at a time and load it into the weather vectors
    }
}
```

```
for (int iyr=0; iyr<2; iyr++)
{
    char myFile[_MAX_PATH];
    char tempData[200];
    char tempNum[10];
    _itoa_s (iniYear+iyr,tempNum,10);

    strcpy_s(myFile, FName);
    strcat_s(myFile, tempNum);

    std::ifstream Rfile(myFile); //open the weather file
    if (Rfile)
    {
        for (int icount=0; icount<23; icount++) //read the first few ↗
            lines of junk
        {
            Rfile.getline(tempData, 200);
        }
        while (!Rfile.eof())
        {
            int myTempInt, myYear;
            double myIr, myMinT, myMaxT, myVP, myWindS, myPre, mySunH;
            Rfile>>myTempInt;
            Rfile>>myYear;
            if (iyr==0)
            {
                if (SetNum==0)
                    Weath0.SetFirstYear(myYear);
                else if (SetNum==1)
                    Weath1.SetFirstYear(myYear);
            }
            Rfile>>myTempInt;
            Rfile>>myIr;
            if (SetNum==0)
                Weath0.AddIrrad(myIr);
            else if (SetNum==1)
                Weath1.AddIrrad(myIr);

            Rfile>>myMinT;
            if (SetNum==0)
                Weath0.AddMinT(myMinT);
            else if (SetNum==1)
                Weath1.AddMinT(myMinT);

            Rfile>>myMaxT;
            if (SetNum==0)
                Weath0.AddMaxT(myMaxT);
            else if (SetNum==1)
                Weath1.AddMaxT(myMaxT);

            //////////////////////////////////////
            //Calculate the thermal time each day
            double Tb = 0;
            double tt(0);
```

```

    if (myMaxT>Tb)
    {
        tt = 0.5*(myMaxT + myMinT) - Tb;
        double PI12, TTB, B2, BA2;
        if (myMinT < Tb)
        {
            PI12 = 24.0 / (2.0*3.14159);
            TTB = PI12*acos(1.0 - 2.0*((Tb - myMinT) / (myMaxT
- myMinT)));
            B2 = Tb*(12.0 - TTB);
            BA2 = (myMaxT + myMinT)*(6.0 - TTB*0.5);
            BA2 = BA2 + PI12*(myMaxT - myMinT)*0.5*sin(TTB /
PI12);
            tt = 2.0*(BA2 - B2) / 24.0;
        }
    }
    if (SetNum == 0)
        Weath0.AddTT(tt);
    else if (SetNum == 1)
        Weath1.AddTT(tt);

    //Calculate the thermal time FOR WHEAT each day
    double WhTb = 0.2;
    double WhTT(0);
    if (myMaxT>WhTb)
    {
        WhTT = 0.5*(myMaxT + myMinT) - WhTb;
        double PI12, TTB, B2, BA2;
        if (myMinT < WhTb)
        {
            PI12 = 24.0 / (2.0*3.14159);
            TTB = PI12*acos(1.0 - 2.0*((WhTb - myMinT) /
(myMaxT - myMinT)));
            B2 = WhTb*(12.0 - TTB);
            BA2 = (myMaxT + myMinT)*(6.0 - TTB*0.5);
            BA2 = BA2 + PI12*(myMaxT - myMinT)*0.5*sin(TTB /
PI12);
            WhTT = 2.0*(BA2 - B2) / 24.0;
        }
    }
    if (SetNum == 0)
        Weath0.AddWhTT(WhTT);
    else if (SetNum ==1)
        Weath1.AddWhTT(WhTT);

```

```

////////////////////////////////////

```

```

Rfile>>myVP;
if (SetNum==0)
    Weath0.AddVapP(myVP);
else if (SetNum==1)
    Weath1.AddVapP(myVP);

```

```
Rfile>>myWindS;
if (SetNum==0)
    Weath0.AddWindS(myWindS);
else if (SetNum==1)
    Weath1.AddWindS(myWindS);

Rfile>>myPre;
if (SetNum==0)
    Weath0.AddPrecip(myPre);
else if (SetNum==1)
    Weath1.AddPrecip(myPre);

Rfile>>mySunH;
if (SetNum==0)
    Weath0.AddsunHours(mySunH);
else if (SetNum==1)
    Weath1.AddsunHours(mySunH);

// myraindur;
//Rfile>>myraindur;

while(Rfile.peek()=='\n') //this bit sorts out some strange ↵
stuff that sometimes happens when there are new lines or tabs ↵
at ends of files
{
    Rfile.ignore(1,'\n');
}
}
Rfile.close(); //release file
}
else
    throw std::logic_error("Error opening weather file");

} //end of year loop

} /// end function to read weather
void ClearWeath(int SetNum)
{
    if (SetNum==0)
    {
        Weath0.~Weather();
    }
    else if (SetNum==1)
    {
        Weath1.~Weather();
    }
    else
    {
        throw std::logic_error("No such weather set");
    }
}
}
```

```
double GetIrrad(int Setnum, int iday)
{
    if (Setnum==1)
    {
        return Weath1.GetIrrad(iday);
    }
    else if (Setnum==0)
    {
        return Weath0.GetIrrad(iday);
    }
    else
    {
        throw std::logic_error("No such weather set");
    }
}
double GetMaxT(int Setnum, int iday)
{
    if (Setnum==1)
    {
        return Weath1.GetMaxT(iday);
    }
    else if (Setnum==0)
    {
        return Weath0.GetMaxT(iday);
    }
    else
    {
        throw std::logic_error("No such weather set");
    }
}
double GetMinT(int Setnum, int iday)
{
    if (Setnum==1)
    {
        return Weath1.GetMinT(iday);
    }
    else if (Setnum==0)
    {
        return Weath0.GetMinT(iday);
    }
    else
    {
        throw std::logic_error("No such weather set");
    }
}
double GetVapP(int Setnum, int iday)
{
    if (Setnum==1)
    {
        return Weath1.GetVapP(iday);
    }
    else if (Setnum==0)
    {
        return Weath0.GetVapP(iday);
    }
    else
```

```
{
    throw std::logic_error("No such weather set");
}
}
double GetWindS(int Setnum, int iday)
{
    if (Setnum==1)
    {
        return Weath1.GetWindS(iday);
    }
    else if (Setnum==0)
    {
        return Weath0.GetWindS(iday);
    }
    else
    {
        throw std::logic_error("No such weather set");
    }
}
double GetPrecip(int Setnum, int iday)
{
    if (Setnum==1)
    {
        return Weath1.GetPrecip(iday);
    }
    else if (Setnum==0)
    {
        return Weath0.GetPrecip(iday);
    }
    else
    {
        throw std::logic_error("No such weather set");
    }
}
double GetsunHours(int Setnum, int iday)
{
    if (Setnum==1)
    {
        return Weath1.GetsunHours(iday);
    }
    else if (Setnum==0)
    {
        return Weath0.GetsunHours(iday);
    }
    else
    {
        throw std::logic_error("No such weather set");
    }
}
double GetTT(int Setnum, int iday)
{
    if (Setnum == 1)
    {
        return Weath1.GetTT(iday);
    }
    else if (Setnum == 0)
```

```
{
    return Weath0.GetTT(iday);
}
else
{
    throw std::logic_error("No such weather set");
}
}
double GetWhTT(int Setnum, int iday)
{
    if (Setnum == 1)
    {
        return Weath1.GetWhTT(iday);
    }
    else if (Setnum == 0)
    {
        return Weath0.GetWhTT(iday);
    }
    else
    {
        throw std::logic_error("No such weather set");
    }
}
}
} //end of namespace
```