A model to simulate yield losses in winter wheat caused by weeds, for use in a weed management decision support system

Laurence R. Benjamin[a,*], Alice E. Milne[a,s], David J. Parsons[b,s], Peter J.W. Lutman[a]

[a] *Rothamsted Research, Harpenden, Hertfordshire, AL5 2JQ, UK*

[b] *Cranfield University, Cranfield, Bedford, MK43 0AL, UK*

([s]*Formerly at Silsoe Research Institute, Wrest Park, Silsoe, Bedford, MK45 4HS, UK*)

***** Corresponding author. Rothamsted Research, Harpenden, Hertfordshire, AL5 2JQ, UK.

Tel.: +44 1582 763133; fax: +44 1582 760981.

E-mail address: laurence.benjamin@bbsrc.ac.uk (L.R. Benjamin).

ABSTRACT

The ‘within-season’ module of the Weed Manager decision support system (DSS) predicts the effect of twelve UK arable weeds on winter wheat yields and profitability. The model and decision algorithm that underpin the DSS are described and their performance discussed. The model comprises: (i) seedling germination and emergence, (ii) early growth, (iii) phenological development, (iv) herbicide and cultivation effects and (v) crop yield loss. Crop and weed emergence are predicted from the timing and method of cultivation, species biology, and the weather. Wheat and weeds compete for resources, and yield losses are predicted from their relative leaf area at canopy closure. Herbicides and cultural control methods reduce weed green area index, improving crop yield. A decision algorithm identifies economically successful weed management strategies based on model output. The output of the Weed Manager model and decision algorithm was extensively validated by experts, who confirmed the predicted responses to herbicide application were sufficiently accurate for practical use. Limited independent data were also used in the validation. The development of the module required integrating novel and existing approaches for simulating weed seedling establishment, plant development and decision algorithm design. Combining these within Weed Manager created a framework suitable for commercial use.

Keywords: Emergence pattern, weed development, weed competition

1. Introduction

Decisions on weed control in winter wheat (*Triticum aestivum L.*) should be a trade-off between economic impact of weeds and control cost. Developing EU legislation (Sustainable Use Directive) is likely to require that pesticide use should be based on a defined need for treatment (CRD, 2009a). The problem of control is complex because weed population and growth varies between sites and years. Generally, weeds are controlled using a combination of cultivations and herbicides. Cultivations can be used to kill emerged weeds pre- or post-drilling or to stimulate a flush of weeds prior to drilling. Herbicide use is even more complex with many commercial products available. Each product targets a subset of weed species with dose and timing affecting control. Products may be applied in mixture and/or sequence, in some cases with synergistic (or antagonistic) effects. Additionally, each herbicide has legal restrictions which limit use to certain times, doses and tank mixtures.

Sustainable weed management requires detailed understanding of weed populations, their effect on yield and methods of control. Simulation models can facilitate this understanding by combining expert knowledge with experimental data and by providing the ability to extrapolate to other years and sites. Here we describe a model, which estimates weed induced yield loss in a winter wheat crop, and its associated decision algorithm. The model simulates the impact of weed control strategies on weed and crop green area index (GAI), which in turn affects crop yield. The objective of the decision algorithm is to produce a list of alternative control strategies that maximise economic margin over weed control costs.

Empirical models have been used to relate crop yield loss to weed density (Cousens, 1985; Pannel et al., 2004) or to early relative leaf areas of weeds and crop (Kropff et al., 1995; van Acker et al., 1997). More complex ecophysiological models have also been developed, which mechanistically simulate competition (Kropff and van Laar, 1993). The model presented in this paper comprises an ecophysiological growth and development model, and an empirical yield loss model. Where possible, established models were used to simulate the different processes, but it was also necessary to develop new approaches. For example, herbicide efficacy depends on weed growth stage (GS). Crop GSs are also needed to accommodate pesticide application restrictions, so models were required to predict phenological development of both wheat and weeds. Additionally, because the effectiveness of herbicides changes with weed growth stage it was very important to simulate the protracted emergence time of each weed species so that on any day a weed species is represented by cohorts at a realistic range of growth stages. Without these the effect of herbicides would be poorly estimated (Wiles et al., 1996).

Simulation models permit the investigation of many alternative weed control scenarios but the main focus of the presented models is to identify strategies that maximise economic margin because this is the primary interest of users. An exhaustive search of all alternatives would be impractical because the search space is large. It is better to use an optimisation algorithm. Many techniques have been developed, such as the genetic algorithm used by Parsons and TeBeest (2004) to optimise winter wheat disease control, or dynamic programming used by Benjamin et al. (2009) to optimise rotational weed control. In our case, the structure of the model and herbicide data meant the most practical approach was to develop an efficient searching strategy based on expert knowledge of weed control, the form of the model, and herbicide and cultivation data. The decision algorithm typically needs to run the model thousands of times, and so throughout the model development we guarded against unnecessary complexity.

The model and decision algorithm described here were developed for the "Weed Manager" decision support system (DSS) (Parsons et al. 2009). This is the first DSS to focus on weed management in UK winter wheat, although cognizance was taken of other weed DSSs (Wiles et al. 1996; Wilkerson et al., 2002; Berti et al., 2003; Rydahl, 2004; Pannell et al., 2004). All approach the problem in different ways depending on their scientific background. Weed Manager was designed for farmers and advisors to investigate their own weed control strategies. Through a graphical user interface (GUI) the user is able to explore the impact of their strategies on economic margin or receive a suggested range of treatments. Weed Manager comprises a within-season module and a rotational module, which simulates weed control over a rotation (Benjamin et al., 2009). The within-season module is designed so that it can be integrated with the rotational module. This is so that factors affecting the long term management of the weed seedbank (essential in any prudent weed control strategy) can be taken into account when planning weed control for the current season. We return to this point in the discussion but throughout the description of our methods we focus on optimising the economic margin of the current crop. Weed Manager is part of ArableDS (Parsons et al., 2004) which is a suite of arable crop DSSs and encyclopaedias. This infrastructure provides the modules with information on pesticide cost, efficacy, mixture information and usage restrictions. It contains local weather and farm data, enabling simulations to be site specific. Copies of the program for Microsoft Windows® are available through www.weedmanager.co.uk**,** or from the authors.

In this paper, we describe the within-season model and decision algorithm for the within-season module of Weed Manager, and explore its performance. We parameterise the models and test them against independent data. Parameters were found for the following weeds; *Alopecurus myosuroides* Huds. (black-grass), *Stellaria media* (L.) Vill. (chickweed), *Galium aparine* L. (cleavers), *Avena fatua* L. (wild-oat), *Anisantha sterilis* (L.) Nevski (barren brome), *Lolium multiflorum* Lam. (Italian ryegrass), *Poa annua* L. (annual meadow-grass), *Chenopodium album* L. (fat hen), *Papaver rhoeas* L. (common poppy) and *Polygonum aviculare* L. (knotgrass), volunteer winter oilseed rape (*Brassica napus* L. ssp. *oleifera*) and volunteer field beans (*Vicia faba L.*).

2. Yield loss model

2.1 Overview of model structure

The model estimates weed induced yield loss in winter wheat for any given weed control scenario, and comprises five sub-models: (i) seedling germination and emergence, (ii) early growth, (iii) phenological development, (iv) herbicide and cultivation effects and (v) crop yield loss. Jointly, they simulate the growth and interaction of winter wheat and arable weeds producing an estimate of the proportional yield loss (Fig. 1).

The starting point for the weed growth simulation is an estimate of the seedbank. This is calculated from the anticipated weed density in the absence of weed control. Users provide this weed plant density by choosing one of four, species-dependent, density ranges. These anticipated densities are used to estimate the initial seedbank by back calculation, which includes adjustments to account for the influence of cultivation practices already carried out (or planned). The calculation of the proportion of seeds that emerge under given cultivation sequences is described in Benjamin et al. (2009).

Seedling emergence is influenced by species, temperature, water, and seasonal changes in dormancy, which interact with seedbed preparation (Forcella, 1998; Finch-Savage et al. 1998). Crop emergence and growth are simulated as a single cohort of seedling emergence at the user defined plant density (plants m^{-2}). Weed species have a more protracted emergence, which is modelled as a function of hydrothermal time (Finch-Savage et al., 1998). Here we captured this variation by simulating eight cohorts emerging over a period of time.

The simulation estimates daily growth stage (GS) and green area index (GAI) of the crop and weeds. This continues until the sum of the individual GAIs exceeds 0.75. This moment is defined as canopy closure. The ratio of the GAI of an individual weed species to the GAI of the crop and weeds at canopy closure is used to estimate the crop yield loss due to that species (Kropff et al., 1995). The total weed induced yield loss is the sum of the yield losses attributed to each individual species. No competition between weed species is assumed, which is a reasonable for most commercial conditions; and also makes the predictions ‘conservative’, over- rather than under-estimating yield losses.

The effect of using herbicides and cultivations on yield loss is modelled by reducing the untreated GAI (calculated at canopy closure) for each weed. The size of the reduction depends on the product used, the dose and the weed cohort GS at the time of application.

As it is not feasible to predict crop yield without taking into account numerous site specific factors that were beyond the scope of the project, we ask the user to provide an estimate of yield in weed free conditions. Yield loss is calculated by scaling this value by the model estimate of proportional yield loss.

In the following sections we describe the model in more detail.

2.2 Climate and astronomical data

The weeds and wheat emerge and grow as a function of daily weather variables and day length. The weather variables, which are provided by the ArableDS environment, are maximum and minimum temperatures, radiation, rainfall and evapotranspiration. The emergence model uses temperature, rainfall, evapotranspiration and photoperiod. The weed and crop growth is modelled using radiation and temperature (as detailed below). Calculation of photoperiod uses the ASTRO procedure and is based on time of year and latitude (Kropff and van Laar, 1993). Users can include their own weather data, or the system will provide data from the nearest national meteorological station.

2.3 Seedling emergence

Our approach assumes the seedling emergence pattern is described by the logistic Equation (1) given as a function of "emergence-day-degrees" accumulated after the initiation of seedling emergence (the "emergence trigger" – see below)

$$n_s(t) = 1/\left(1 + \exp\left(-\beta\left(\sum_{x=t_d}^{t} D_s(x) - \delta\right)\right)\right) \tag{1}$$

where $n_s(t)$ is the proportion of seedlings that have emerged, t is day number, t_d is the emergence trigger day, δ and β are species-dependent parameters, and D_s (t) is the emergence day-degrees on day t. The variable D_s is defined

$$D_s(t) = T_d(t) f_m(t) f_d(t) \tag{2}$$

where T_d is the mean temperature above base (0ºC), f_m is the moisture factor and f_d is the dormancy factor (Forcella, 1998).

The emergence trigger is defined either as harvest date of the previous crop or the date of ploughing, if it has occurred. This is based on the assumption that ploughing buries and destroys seeds that have germinated and seedlings that have emerged, but brings another set of seeds to the surface, which start to emerge. The model assumes that the number of seeds being brought to the surface will be similar to the number buried. This simplifying assumption is made in the absence of field specific data on the distribution of seeds in the soil profile. Non-inversion cultivations have a less extreme effect on seed distribution in the soil and so the emergence trigger of harvest date is retained where these cultivations are used.

2.3.1 Soil moisture factor

This assumes that soil moisture content is between the wilting point and field capacity. Allen et al. (1998) reported that the difference in moisture content between these points was up to 0.2 m^3 m^{-3} for loams and clays. The model considers the top 100 mm, within which germination occurs, and assumes the soil is at wilting point at the emergence trigger. We make this assumption because the trigger is either harvest or ploughing, which are typically conducted in dry weather and the model is dealing with the layer of soil that dries most rapidly. The model accumulates the difference between rainfall and potential evapotranspiration (mm), constrained within the range 0 (wilting point) to 20 mm (field capacity). The soil moisture factor f_m is 1.0 if the soil moisture value is greater than 5mm, otherwise it is 0.0.

2.3.2 Dormancy factor

The dormancy factor, f_d, is a species-dependent function of the day of the year in the range 0 – 1. To define the dormancy factor, the numbers of seedlings established each month were taken from Mortimer (1990) (*A. myosuroides*, *S. media*, *G. aparine*, *A. fatua*, *P. annua*, *C. album*, *P. rhoeas* and *P. aviculare*) and Froud-Williams (1983) (*A. sterilis*). *Lolium multiflorum* was assumed to have the same dormancy characteristics as *A. sterilis*, whilst *B. napus* and *V. faba* have no dormancy. For each species, the number emerging each month was expressed as a proportion of the total number of seedlings emerging per year. This emergence pattern is the result of all of the factors in Equation (1), so several simplifying assumptions were required to estimate the dormancy factor. The seasonal temperature and soil moisture cycles were not published for the Froud-Williams (1983) and Mortimer (1990) data, so these were accounted for by standardising the emergence of each species using *P. annua*. This has no seasonally affected dormancy, so its monthly emergence pattern can be attributed entirely to seasonal changes in soil temperature and soil moisture. For each month, the ratio of emergence of *P. annua* in July (the month with the greatest emergence) to the monthly emergence was taken as a weighting factor applied to the monthly proportional emergence of other weed species. A cubic polynomial was fitted to these values for each species and the slope of this cubic polynomial for any day of the year was scaled to lie in the range [0, 1], to define the dormancy function

2.3.3 Parameterising the emergence pattern equation

Seedling emergence counts for winter wheat, *A. myosuroides*, *G. aparine* and *S. media* had been recorded at six sites, in three seasons, in a research project reported by Ingle et al. (1997) approximately weekly for 100 days after sowing, along with daily maximum and minimum temperatures. The drilling dates were late September or early October in all cases. The daily temperature, precipitation and evapotranspiration needed to calculate accumulated emergence-day-degrees for the Ingle et al. (1997) data were provided by J. Storkey (personal communication). Equation (1) was fitted to each of the three species included in the 'Ingle' experiments separately using FITCURVE (Genstat, 2002) (Table 1). The range of temperatures during the experimental period was not sufficiently broad to allow the day-degrees base temperature to be estimated accurately, and so it was assumed to be 0^oC (estimated from Finch-Savage et al. (1998)). The agreement between observed and fitted data was close (86, 88, 85 and 82% variance accounted for in adjusted R^2 for *A. myosuroides, S. media, G. aparine* and wheat, respectively). The data for *A. myosuroides* are presented in Fig. 2. In the absence of species specific data for the other weed species, emergence was extrapolated from the behaviour of these three; for example the grass weeds *L. multiflorum, A. sterilis* and *P. annua* followed *A. myosuroides*.

2.3.4 Implementing emergence patterns in the model

The model of emergence given by Equation (1) estimates the accumulated daily weed seedling emergence. To model the subsequent development of each seedling would make the model run time unacceptably long. Therefore we simplified the method whilst still retaining the qualitative nature of the emergence patterns. For wheat, seedlings are assumed to emerge δ emergence-day-degrees after sowing. Weed emergence is simulated over a spread of time by dividing the emergence period of each weed species into eight cohorts of equal density. Eight was judged to be the lowest number of cohorts that adequately captured the period of emergence. The number of seedlings in each cohort is calculated by dividing the expected number by the number of cohorts that emerge after drilling.

The simulation accounts for seedbed preparation stimulating the emergence of weeds. In all preparation methods one cohort germinates at drilling and emerges 80 emergence-day-degrees later (Finch-Savage et al. 1998). The other seven cohorts germinate at specified intervals from the emergence-trigger (based on the theoretical emergence pattern above).

The accumulated emergence-day-degrees, $H_e(i)$, between the emergence-trigger and emergence date for each cohort (i = 2, …8) is defined by rearranging Equation (1) to give

$$H_e(i) = \delta - \frac{1}{\beta} \ln\left(\frac{1 - f(i-1)}{f(i-1)} \right) \tag{3}$$

where for direct drill $f(i) = (0.125, 0.25, 0.375, 0.5, 0.625, 0.75\ \ 0.875)$. For other cultivation sequences (ploughing and non-inversion cultivation) the soil disturbance breaks the dormancy of some seeds bringing forward germination of cohorts i = 3,…,8. For simplicity we assume that cohort 3 emerges at the same time as cohort 2 and cohorts 4 – 8 emerge when cohorts 3 – 7 would under a direct drill scenario, thus $f(i) = (\,0.125, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75)$.

2.4 Phenological development

Herbicide efficacy depends on weed GS, and pesticide application restrictions are often given in terms of the GS of the crop. Although growth was only simulated up to canopy closure, herbicides could be applied throughout the season from drilling to harvest. Therefore we needed to model the phenological development of weeds and crop up until maturity. We used the Zadoks GS scale for graminaceous weeds and wheat (Zadoks et al., 1974). Growth stages from GS30 to maturity (GS92) are defined by Milne et al. (2003). The beginning of germination (H_g) (GS0), is defined in emergence-day-degrees by

$$H_g(i) = \max\{H_e(i) - 80.0, 0\} \tag{4}$$

Between germination and the day of emergence (t_s) the GS (Z) on day t is

$$Z = 10 \sum_{s=t_g}^{t} D(s) / \sum_{s=t_g}^{t_s} D(s) \tag{5}$$

where D is day-degrees. After emergence, $Z = 10$ until the first leaf is formed. A new leaf appears when the accumulated day degrees from the appearance of the previous leaf exceed the species specific phyllochron. The value of Z increases from 11 to 14 with the appearance of first to fourth leaf. Once four leaves have been produced tillering commences (GS21–29). Tillers appear every 100 day ^{o}C (based on expert opinion) until main stem extension (GS 30) is initiated.

A similar approach is taken for broad-leaved weeds with GSs after emergence based on the number of leaves on the entire plant. Unlike graminaceous weeds, branching (the equivalent of tillering) does not directly affect the GS code. The number of leaves produced per phyllochron may be more than one (e.g. a pair of opposite leaves). Flower buds are produced when a species-specific number of day degrees have accumulated.

2.5 Growth and competition

The growth of each species from emergence to canopy closure is simulated using the ecophysiological model INTERCOM (Kropff and van Laar, 1993). The height and leaf area of the crop and weeds determine their daily light interception, and the consequent increase in dry matter is partitioned to the different plant organs. The increase in GAI is calculated from the specific leaf area. The initial GAI of each weed cohort and the crop is based on the green area per seedling at the time of full hypocotyl or cotyledon expansion and density. Where this initial seedling green area is not known the value is estimated as the product of: for grasses, the green area per *A. myosuroides* seedling (35 mm^2) and the ratio of the species seed weight to the seed weight of *A. myosuroides* (1.1 mg); and for broad-leaved species, the product of the green area per *S. media* seedling (31 mm^2) and the ratio of the species seed weight to the seed weight of *S. media* (0.8 mg) (Storkey, 2001).

Photosynthate supply or temperature can limit plant growth (Benjamin and Park, 2007). To estimate which of these is most limiting, daily increase in GAI is calculated in two ways: firstly, from the above calculations of dry matter (based on INTERCOM) and secondly from a simple temperature based exponential model (Storkey and Cussans, 2000). The daily increase in GAI is taken as the lower of the two values. For weed species that are not winter hardy, there is a daily loss of 90% of total GAI whenever the minimum air temperature falls below -5^{o}C. This is necessary to ensure the model does not predict yield loss from autumn-emerging weeds that do not survive British winters.

The simulation commences on the date of emergence of the first cohort of the weed or the crop (which ever is the earliest), and further weed cohorts are included as the simulation proceeds to canopy closure (GAI = 0.75).

2.6 Crop yield loss

The yield loss (t ha $^{-1}$) associated with a weed species is

$$Y_L = \frac{YqL_w}{1+L_w(q-1)} \qquad (6)$$

where Y is crop yield (t ha $^{-1}$) in weed-free conditions, q is the weed species dependent damage coefficient. L_w is

$$L_w = \frac{GAI_w}{GAI_w + GAI_c} \quad (7)$$

(Kropff et al., 1995), where GAI_w is the GAI of weed *w* and GAI_c is the crop GAI at canopy closure. Values for *q* were derived from our own experiments and from the published literature and were 2.55 for *A. myosuroides*, 0.6 for *S media* and 23.9 for *G. aparine*. The weeds are assumed to act independently of one another. That is to say, it is assumed that one weed's growth does not suffer from the competitive effects of another. Therefore, the total weed-induced yield loss is calculated as the sum of the yield losses attributed to each weed species. The total yield loss is not allowed to exceed the weed-free crop yield.

2.7 Weed control (*herbicide and cultivation effects*)

The effect of using herbicides and/or mechanical cultivations on yield loss is modelled by reducing the untreated GAI of each weed cohort calculated at canopy closure. The reduction depends on the product (the term "product" includes cultivations and herbicides) efficacy. The efficacy *e* of a product against a weed cohort will depend on the weed species, the dose applied and the GS of the cohort at the time of application. The model of herbicide control is not mechanistic. The effect of each weed control measure, be it conducted before or after canopy closure, is reflected in a reduction in GAI at canopy closure. The effect of timing of control on yield is implicit in the efficacy. In the majority of cases, late application will result in reduced efficacy. Therefore, the model will favour early treatment, but there will be a bias towards some under-prediction of yield loss at later applications because the model does not fully account for greater duration of weed competition.

The product efficacy data are stored in a database which is accessed by the model. They take a similar form to herbicide label data, with efficacies given for fixed doses against weed species at consecutive GS ranges. For grass weeds the Zadoks GS ranges are $0-7$, $8-10$, $11-13$, $14-21$, $22-29$, $30-31$, $32-39$, $40-45$ and $46-93$; for broad-leaved weeds the ranges are pre-emergence, pre-emergence – cotyledons, cotyledons – 2 leaves, $2-4$, $4-6$, $6-8$, and 8 leaves – flowering. The efficacies are categorised as resistant, moderately resistant, moderately sensitive, sensitive and complete kill, mapping to e=0.01, 0.51, 0.76, 0.91 and 1.0, respectively. These values are similar to those published by CRD (2009b) for herbicide registration. Published and unpublished (but manufacturer supported) product information was used to assign efficacies to each weed species, GS and product combination (D. H. K. Davies, personal communication).

If a single product is applied to a weed, the treated GAI of the *j*th cohort is obtained by multiplying the untreated GAI by the product efficacy, *e*. If a product mixture is applied it is treated in one of two ways. If the product mixture (including product plus adjuvant) is known to be synergistic then the combination is treated as a pseudo product with its own efficacy data. Otherwise the combined efficacy *E*, of products either in mixture, sequence or both is calculated by:

$$E = 1 - \prod_{i=1}^{n} (1 - e_i) \tag{8}$$

where e_i is the efficacy of the i^{th} product against the weed cohort at the GS at which it was applied, and *n* is the number of products in the control programme.

2.8 Variability

There is always some uncertainty in prediction. This is due to, among other factors, error in the seedbank estimation and unknown future weather. Therefore the model prediction of weed induced yield loss is presented to the user as a range of values, indicating the variability associated with the prediction. We assume that most variability arises from uncertainty associated with estimating weed and crop density. The users define the weed and crop populations from a set of density ranges. The mean expected yield loss is calculated using the means of the density ranges for weed and crop. The greatest/least possible yield loss is calculated using the lower/upper bound of the crop density and the upper/lower bound of the weed density.

3. The decision algorithm

The decision algorithm suggests a list of the most robust weed control strategies for a given scenario. The scenario comprises weather, site, sowing date, weed list and any cultivations and herbicides applied to date in the season.

The algorithm incorporates rules on cultivation practices and timing and dose of herbicides, ensuring only legally acceptable and practical strategies are suggested. These rules are either "restrictions data", which are part of the legal registration process, or "recommendations for effective use" and are defined by the herbicide manufacturers and marketers. Most are on the product label. Restrictions and recommendations data contain "do not mix" rules prohibiting dangerous or antagonistic tank mixes. There are also restrictions on pre-sowing sequences of cultivations to ensure an appropriately prepared seedbed. All of the above rules are contained in the ArableDS and Weed Manager databases. Each cultivation and herbicide programme is validated against the rules.

The decision algorithm aims to maximise the margin, *M*, over weed control costs

$$M = (Y - Y_L)g - P_H - P_C \tag{9}$$

where Y is the expected weed-free crop yield, Y_L is the weed induced yield loss, g is the grain price, P_H is the cost of the herbicide programme and P_c is the cost of the cultivation programme.

To ensure the algorithm reaches a solution within a few minutes (a time acceptable to users) the slowest parts of the model are run as few times as possible (otherwise reaching a solution could take several hours). These are calculating emergence patterns and growth to canopy closure. The emergence pattern depends on the pre–sowing cultivation programme (see Fig. 1) and once the pattern is established subsequent weed control treatments have no effect on GS estimates. The decision algorithm exploits this by minimising the number of cultivation combinations to be tested and calculating the growth stages for each only once.

If the sowing date is prior to the current date, then it follows that the pre-sowing cultivation programme has been defined by the user. Otherwise, the suggested control strategies include pre-sowing cultivations. To minimise the number of cultivation combinations tested, the system selects up to three pre-sowing cultivation programmes (described below). For each cultivation programme the model is run to canopy closure and the untreated GAIs are stored. A list of valid herbicide and post-sowing cultivation programmes is generated (described below) and their effects on the weed GAI are calculated using Equation (8). These are applied to the untreated GAI and the revised GAIs are used to calculate the weed induced yield loss (Equation 6) and margin (Equation 9). The weed control programmes are sorted to remove poor solutions and repetitions of very similar programmes and the top 20 are presented to the user. This produces a short list of diverse solutions.

3.1 Defining the pre-sowing cultivation programme

The system contains data for eight pre-sowing cultivations (mouldboard plough, spring tine, harrows, rollers, powered harrows, heavy tines, discs, heavy disc) as well as drilling and direct drilling. These are used in combination to prepare the seed bed and sow the wheat. We term such a series of activities a pre-sowing cultivation programme. If the current date is before sowing and the user has not identified any preferred options, a maximum of three pre-sowing cultivation programmes are selected: nominally non-inversion, ploughing and direct drill. The non-inversion sequence starts with the primary cultivation (1) on the day after the current date and follows this with secondary cultivation (2) on the day before drilling. The first cultivation stimulates weed emergence and the second removes many of those that have emerged. Hence the maximum amount of time is left between cultivations (Pannell et al., 2004). This sequence is run for all valid combinations of cultivations 1 and 2 (tested against database information on timing and which combinations of cultivations acceptably prepare the seedbed). The cultivation plan that gives the highest margin defines the non-inversion programme. For ploughing, cultivation 1 is mouldboard plough two days before drilling (removing most of the germinated weeds) and cultivation 2 is harrowing the next day. The direct drill programme sows the crop without any pre-sowing soil cultivations. If primary cultivations have already been done these effectively define cultivation 1 and only cultivation 2 is selected by the algorithm. In this case, the model is run with all valid options for cultivation 2 and the one that gives the highest margin is selected. As stated above this method results in a maximum of three different pre-sowing cultivation programmes, which are taken forward and investigated with valid herbicide combinations as described below. To ensure the optimisation reaches a solution in a few minutes it was necessary to define the timings for the non-inversion and ploughing sequences. These were based on one of several possible practical approaches. The chosen timings will not be the best in all scenarios, but will produce robust solutions. The users are still able to define other sequences that can be taken forward to the next step of the optimisation should they wish to.

3.2 Defining the herbicide and post-sowing cultivation programme

There are many herbicide products available and users can, if they wish, limit the herbicide selection by only including products that are available on their farms. The season is split into four consecutive treatment periods; “pre-emergence” (before wheat GS 9), “autumn” (between GS 9 and 1st January), “spring” (between 1st January and GS 90) and “desiccant” (period after GS 90). In each period there is only one application of product/mixtures. In each period the timing for each product/mixture that gives the least yield loss is evaluated and saved to a list. The lists are reduced by removing products/mixtures that have lower efficacy against the target weeds than cheaper products/mixtures in the list. All valid combinations of the reduced lists are evaluated forming a list of “viable programmes”, and up to 20 of the best performing programmes are presented to the user (as described above).

4. Model validation

Some experimental data were available but these were insufficient to validate the model and decision algorithm fully, so much of the validation was done using expert agronomic opinion. Field and research weed scientists associated with the project but not directly involved in model development, examined a wide range of outcomes from the model, with the different weed species, cultivation practices and herbicides, and assessed whether the predictions were agronomically sound. This resulted in many improvements. Several independent data sets from the UK were also found that could be used for partial validation.

These included published papers and unpublished research carried out by consortium members. The work focused on assessing predicted crop yields arising from uncontrolled infestations of target weeds, as these responses were more likely to identify problems with the predictions but some herbicide performance data were also identified.

Independent data were found for *S. media*, *G. aparine*, *A. fatua* and *A. myosuroides*. As far as possible, the published agronomic data were used as the basis for the predictions. As these data spanned several decades, we were unable to access the associated weather data. Consequently, we used standardised ArableDS regional climatic data (Parsons et al., 2009).

4.1 Predicting yield losses from uncontrolled weeds

4.1.1 Broad-leaved weeds (S. media *and* G. aparine)

Wheat yield responses to *S. media* were determined from three experiments (Lutman unpublished data, 2006). The model consistently over-estimated the crop response to competition from this weed, especially at higher densities at Rothamsted (Table 2). The two experiments on *G. aparine* showed contrasting yield responses (Wright and Wilson, 1992). In trial Bristol 1, there was little yield loss from the weed, whilst the model predicted considerable losses. Wright and Wilson commented on the surprising lack of yield loss from the *G. aparine* and attributed this to a summer drought that reduced its competitive effect. In contrast, in Bristol 2 the yield losses were higher and within the range the model predicted.

4.1.2 Grass weeds (A. fatua *and* A. myosuroides)

Two experiments (Oxford 1 and 2) measured the response of winter wheat to competition from *A. myosuroides* (Wilson, 1980). In Oxford 1, predicted yield loss was close to the actual response (Table 2), whilst in Oxford 2 it was less than predicted. Wilson attributes the low yield loss in Oxford 2 to the 'profuse late summer vigour of the wheat'. In the four *A. fatua* experiments, the model was within 0.6 t ha^{-1} in two experiments (Bristol 4 and Oxford 4), underestimated the response in Bristol 3 and overestimated it in Oxford 3 (Wilson et al., 1990; Wright and Wilson, 1992). The two Oxford data sets were from the same experiment, but with differing crop densities. The results suggest the model was overreacting to the low crop density in Oxford 3 and if it is increased by one band (i.e. from 100–149 to 150–199 wheat plants m^{-2}) the predictions are much closer to the actual yields. The more pronounced yield losses in the Bristol 3 experiment, which was done in the same season as Bristol 1, may also be associated with the summer drought, as the crop was unable to compensate for the early competition exerted by the *A. fatua*.

4.2 Evaluation of predicted crop yield responses to the control of A.myosuroides

The previously discussed experiments on *A. myosuroides* (Wilson, 1980) also included results from November applications of isoproturon. These achieved good weed control and yields increased (Table 3). Predictions for Oxford 1 were within 0.7 t ha^{-1} of the observed yield and those for Oxford 2 continued to over-estimate yield losses (as discussed above).

A third experiment evaluated herbicidal control of metabolic resistant *A. myosuroides* at ADAS (Boxworth). It compared three treatments (classed as early, late and full) and an untreated control. The model under-estimated the yield loss in the absence of weed control, but predictions improved with increased control. The prediction with the least effective (early) treatment was least accurate, reflecting the under-estimate of the response of the untreated.

5. Discussion

The model and decision algorithm were developed for the Weed Manager DSS, and this purpose determined their design. It meant achieving a balance between being sufficiently complex so that key parts of the biological mechanism were described, parsimony and model run times of a few seconds (important for the decision algorithm). Established models were used where possible. For example, yield loss was based on well-established models relating yield loss to relative crop and leaf area (Kropff et al., 1995) and seedling emergence was based on hydrothermal models of seedling establishment (Finch-Savage et al., 1998; Forcella, 1998). However, it was also necessary to develop new modelling approaches to certain aspects of weed development: for example, the effect of seed dormancy, spread of weed seedling emergence, and growth stage progression. Where sufficient data were not available to define parameters for the novel parts of the model, expert opinion and logical extrapolation were used. In particular there were insufficient data to estimate the day-degree requirement for seed germination and seedling emergence or their base temperatures and, for some species, initial seedling green area. Similarly, the stimulation of seedling emergence due to soil disturbance was simulated by advancing a cohort to be a specified thermal time after seedbed preparation. Since the time of development of the DSS new data have become available (J. Storkey, personal communication) and so it may now be possible to estimate these parameters more accurately. Our concerns to minimise runtime led to the pragmatic decision to base estimates of yield loss on the relative calculated GAI of the crop and the weed at canopy closure. It would have been biologically sounder to incorporate the impact of the time of control on weed competition more mechanistically, but with computer power at the time of development was impractical. Increased computer power in the future may provide opportunities to re-evaluate this. Despite these shortcomings, expert assessment of the models concluded that they performed sufficiently well and were fit for purpose.

For legal liability reasons, the system uses only approved recommended rates of herbicide products. Therefore, dose flexibility is not as great as in some other weed DSSs (e.g. Rydahl, 2004). An advantage of our method is that herbicide parameter updates are straightforward, as they can be extracted from labels. However, this approach requires a large number of herbicide product parameters, unlike the more parsimonious approach of parameterising active ingredients (see Milne et al., 2007).

The decision algorithm also proved an unwitting critic of the model as, during the system development, it suggested mathematically correct, but biologically flawed solutions. This led to an improved description of biological mechanisms important to weed control, in particular, the need to account for the protracted emergence of weed species. The decision algorithm was tested by experts who concluded the results were sound (Parsons et al., 2009).

The field trials indicate that in the absence of weed control, the model tends to over-estimates yield losses from weeds. However, because of large variation in the data we are cautious with our conclusions. Taking into account the variability in the field data, yield losses were over-estimated in five trials, under-estimated in two and were reasonably accurate in four. The over-estimation mainly affected the *S. media* results and this systematic error requires attention. From a farming viewpoint, this over-estimation is a lesser error, as it is risk averse. In three of the 11 trials, extreme summer weather resulted in poor predictions of yield loss, as they had influenced the competitive characteristics of the species concerned. The drought in experiments B1 and B3 had had contrasting effects. It had reduced the competitive effect of *G. aparine*, as this late maturing species was unable to develop its normally highly competitive canopy in late summer. In contrast the drought increased the competitive impact of *A. fatua*, as this earlier maturing species was able to exert its full competitive impact on the crop, whilst the crop was unable to recover in the latter part of the summer. These issues highlight problems associated with predicting yield loss early in the season, when variable weather events ensue. Weed Manager is designed to be run throughout the season, with weather data and weed observation updates. Consequently, as the season progresses, predictions should improve. The limited validations of herbicide performance (Table 3) indicate that where weed control is high the model's predictive ability is better than in the absence of control. This is encouraging because we would expect the variability in response to herbicide treatment to reduce with increased control, and so should be more accurate.

The within-season module discussed in this paper has been presented as a decision support module that is concerned only with the current cropping season. This is often not the most practical approach and weed control should ideally take a more long term view if the weed seedbank is to be kept at a manageable level. This is the focus of the rotational module (Benjamin et al 2009), which accompanies the within-season module in the Weed Manager DSS. The two systems have been designed to be compatible. The long term module can be used to estimate the percentage kill needed to keep a weed at a manageable level over a rotation. The within-season module estimates the expected kill of each weed under a given scenario and displays it to the user so that they can see if their targets have been met. In future developments we plan that the user will be able to define a minimum percentage kill (for example that suggested by the rotational system) that the optimisation algorithm must aim to achieve. Solutions which do not achieve this target will be removed from the list of viable programmes (described above).

Weed Manager was developed as a tactical DSS for farmers and advisors but also has educational value, illustrating the complex interactions between weed biology, cultivation practices and weed control. For example, the within-season module provides a valuable tool to explore and illustrate the complex interactions between the range of development stages of weeds, their competitive effects and vulnerability to control measures. Development is still needed, to increase the number of weeds and to validate the results of the species currently included.

Acknowledgements

Defra (through Sustainable Arable LINK LK0916) sponsored this project, with HGCA, BASF, Bayer CropScience, Dow AgroSciences, DuPont, and Syngenta. We acknowledge contributions of staff from ADAS, Rothamsted Research, Silsoe Research Institute and the Scottish Agricultural College, particularly Jonathan Storkey, Audrey Mayes and John Cussans. Rothamsted Research receives grant-aided support from the Biotechnology and Biological Sciences Research Council (BBSRC).

References

Allen, R.G., Pereira, L.S., Raes, D., Smith, M., 1998. Crop evapotranspiration - Guidelines for computing crop water requirements - FAO Irrigation and drainage paper 56, FAO - Food and Agriculture Organization of the United Nations. Rome, 1998, http://www.fao.org/docrep/X0490E/X0490E00.htm, date accessed 11 December 2009.

Benjamin, L.R., Park, S.E., 2007. The Conductance model of plant growth and competition in monocrop and species mixtures: a review. Weed Res. 47, 284–298.

Benjamin, L.R., Milne, A.E., Parsons, D.J., Cussans, J., Lutman, P.J.W., 2009. Modelling weed management over a rotation in the UK using stochastic dynamic programming to create a decision tool. Weed Res. 49, 207–216.

Berti, A.F., Bravin, F., Zanin, G., 2003. Application of decision-support software for postemergence weed control. Weed Sci. 51, 618–627.

Cousens, R., 1985. A simple model relating yield loss to weed density. Ann. Appl. Biol. 107, 239–252.

CRD, 2009a. Proposal for a regulation of the European parliament and of the council establishing a framework for Community action to achieve the sustainable use of pesticides. Summary of provisions. Health and Safety Directorate: Chemical Regulation Directorate – Pesticides. York, United Kingdom available at http://www.pesticides.gov.uk/uploadedfiles/Web_Assets/PSD/Outcomes_paper_-_Sustainable_Use_Directive_(Jan_09).pdf (accessed July 09).

CRD, 2009b. Data requirements handbook. Chapter 8: Guidance on efficacy requirements. pub. Health and Safety Directorate: Chemical Regulation Directorate – Pesticides, York, United Kingdom, available at: http://www.pesticides.gov.uk/psd_pdfs/registration_guides/data_reqs_handbook/efficacy.pdf (accessed July 09)

Finch-Savage, W.E., Steckel, J.R.A., Phelps, K., 1998. Germination and post-germination growth to carrot seedling emergence: predictive threshold models and sources of variation between sowing occasions. New Phytol. 139**,** 505–516.

Forcella, F., 1998. Real-time assessment of seed dormancy and seedling growth for weed management. Seed Sci. 8, 201–209.

Froud-Williams, R. J., 1983. The influence of straw disposal and cultivation regime on the population dynamics of *Bromus sterilis*. Ann. Appl. Biol. 103, 139–148.

Genstat, 2002. Genstat, 6th Edition, VSN International Ltd, Hemel Hempstead, United Kingdom.

Ingle, S., Blair, A.M., Cussans, J.W., 1997. The use of weed density to predict winter wheat yield. Aspects of Applied Biology 50, Optimising cereal inputs: its scientific basis.

Part 2 - crop protection and systems, pp. 393–400. Association of Applied Biologists, Wellesbourne, UK.

Kropff, M.J., Van Laar, H.H., 1993. Modelling crop-weed interactions, CAB International, Wallingford, UK.

Kropff, M.J., Lotz, L.A.P., Weaver, S.E., Bos, H.J., Wallinga, J., Migo, T., 1995. A two parameter model for prediction of crop loss by weed competition from early observations of relative leaf area of the weeds. Ann. Appl. Biol. 126, 329–346.

Milne, A., Paveley, N., Audsley, E., Livermore, P., 2003. A Wheat Canopy Model For Use In Disease Management Decision Support Systems. Ann. Appl. Biol.143, 265–274.

Milne, A.E., Paveley, D., Audsley, E., Parsons, D.J., 2007. A model of the effect of fungicides on disease-induced yield loss, for use in wheat disease management decision support systems**.** Ann. Appl. Biol. 151, 113–125.

Mortimer, A.M., 1990. The biology of weeds. In: Hance, R.J. and Holly, K. (Eds), Weed control handbook: principles, pp. 1–43. Blackwell Scientific Publications, Oxford, UK.

Pannell, D.J., Stewart, V., Bennett, A., Monjardino, M., Schmidt, C., Powles, S.B., 2004. RIM: a bieconomic model for integrated weed management of *Lolium rigidum* in Western Australia. Agric. Systems 79, 305–325.

Parsons, D.J., Te Beest, D., 2004. Optimising fungicide applications on winter wheat using genetic algorithms. Biosystems Eng. 88, 401–410.

Parsons, D. J., Benjamin, L.R., Clarke, J., Ginsburg, D., Mayes, A., Milne, A.E., Wilkinson, D.J., 2009. Weed Manager – A model-based decision support system for weed management in arable crops. Comput. Electron. Agric. 65, 155–167.

Parsons, D., Mayes, A., Meakin, P., Offer, A., Paveley, N., 2004. Taking DESSAC forward with the Arable Decision Support Community. Aspects of Applied Biology 72**,** Advances in applied biology: providing new opportunities for consumers and producers in the 21st century, pp. 55-66. Association of Applied Biologists, Wellesbourne, UK.

Rydahl, P., 2004. A Danish decision support system for integrated management of weeds. Aspects of Applied Biology, 72, Advances in applied biology: providing new opportunities for consumers and producers in the 21st century, pp. 43–53. Association of Applied Biologists, Wellesbourne, UK.

Storkey, J., 2001. A physiological approach to understanding weed competition. PhD Thesis, Nottingham University, UK.

Storkey, J., Cussans, J.W., 2000. Relationship between temperature and the early growth of winter *Triticum aestivum* and three weed species. Weed Sci. 48, 467–473.

Van Acker, R.C., Lutman, P.J.W., Froud-Williams, R.J., 1997. Predicting yield loss due to interference from two weed species using early observations of relative weed leaf area. Weed Res. 37, 287–299.

Wiles, L.J., King, R.P., Schweizer, E.E., Lybecker, D.W., Swinton, S.M., 1996. GWM: General Weed Management Model. Agric. Systems 50, 355–376.

Wilkerson, G.G., Wiles, L.J., Bennett, A.B., 2002. Weed management decision models: pitfalls, perceptions, and possibilities of the economic threshold approach. Weed Sci. 50, 411–424.

Wilson, B.J., 1980. The effect of yield of mixtures and sequences of herbicides for the control of *Alopecurus myosuroides* and broad-leaved weeds in winter cereals. Weed Res. 20, 65–70.

Wilson, B.J., Cousens, R.D., Wright, K.J., 1990. The response of spring barley and winter wheat to *Avena fatua* population density. Ann. Appl. Biol. 116, 601–609.

Wright, K.J., Wilson, B.J., 1992. Effects of nitrogen fertiliser on competition and seed production of *Avena fatua* and *Galium aparine* in winter wheat. Aspects of Applied biology, 30**,** Nitrate and farming systems, pp. 381–386. Association of Applied Biologists, Wellesbourne, UK.

Zadoks, J.C., Chang, T.T., Konzak, C.F., 1974. A decimal code for the growth stages of cereals. Weed Res. 14, 415–421.

Figure 1. A diagram of the model structure. The rectangular shapes represent each of the sub models. Where appropriate we have indicated the origin of each model in the rectangle. The oval shapes represent input data provided either by the user or the ArableDS environment. The output from each sub-model is described by the bold text under each sub-model and bold arrows indicate where this feeds into another sub-model.

Figure2 The cumulative number of emerged *A. myosuroides* seedlings at six sites: (a) Boxworth, (b) Bridgets, (c) Drayton, (d) High Mowthorpe, (e) Rothamsted and (f) Woburn (Cussans unpublished data; Ingle et al., 1997). Symbols are the observed counts and lines are the simulated counts using Equation (1). ○ ▬▬ ○ 1994-5, □ - - - □ 1995-6 and Δ…….Δ 1996-7.

Table 1

Equation (1) parameter values for β and δ fitted using seedling emergence data from Ingle et al., (1997) and Cussans J. unpublished data, ± standard error.

Parameter	Species			
	Wheat	*Alopecurus myosuroides*	*Stellaria media*	*Galium aparine*
β ($^{o}C^{-1}$)	0.0174±0.00280	0.0261±0.00388	0.0263±0.00293	0.0228±0.00252
δ (^{o}C)	159±9.4	112±3.9	103±4.0	142±6.9
number of observations	138	150	144	156

Table 2
Weed induced yield loss in the absence of weed control from independent research reports and the associated predictions using the Weed Manager model.

Weed species	Site	Sowing date	Validation data			Weed Manager predictions	
			Weed density (plants m^{-2})	Crop yields (t ha^{-1})	sed	Weed density range	Crop yields (t ha^{-1})
Stellaria media	ADAS Boxworth 1	11 October	48	7.3	0.47	16-60	6.9
			107	7.3		61-180	5.7
			243	7.2		181-230	5.4
(Lutman unpublished 2006)			Weed-free	8.8			
	Rothamsted	18 October	31	5.7	0.65	16-60	4.7
			90	6.0		61-180	3.8
			280	5.2		181-230	3.7
			Weed-free	6.7			
	ADAS Boxworth 2	2 October	30	7.8	0.50	16-60	7.2
			113	7.1		61-180	6.5
			Weed-free	8.1			
Galium aparine	Bristol 1	September	14	6.3	0.71	9-24	4.8
			44	5.8		25-74	3.0
			Weed-free	6.6			
(Wright and Wilson 1992)	Bristol 2	September	15	5.0	0.64	9-24	6.2
			49	2.5		25-74	3.8
			Weed-free	8.4			
Alopecurus myosuroides	Oxford 1	Mid-October	32	6.7	0.52	26-100	6.1
			Weed-free	7.4			
(Wilson 1980)	Oxford 2	Mid-October	113	7.4	0.35	101-250	5.3
			Weed-free	7.9			

Avena fatua	Bristol 3	September	7	3.8	0.71	4-12	5.8
			28	2.0		13-48	4.1
(Wright and Wilson 1992)			Weed-free	6.7			
	Bristol 4	September	4	7.0	0.64	4-12	7.6
			27	5.7		13-48	5.3
			Weed-free	8.7			
Avena fatua	Oxford 3*	4 October	25	6.0	na	13-48	4.5
			75	4.6		49-98	2.9
(Wilson et al. 1990)			Weed-free	7.6			
	Oxford 4*	4 October	25	6.7	na	13-48	6.4
			75	5.7		49-98	5.1
			Weed-free	7.7			

* Oxford 3 – crop density 134 plants m^{-2}; Oxford 4 crop density 443 plants m^{-2}

Table 3

Crop yield responses to application of herbicides to control A. *myosuroides* and corresponding predictions using the Weed Manager model

Site	Weed density (plants m^{-2})	Herbicide treatment	Crop yields (t ha^{-1})		
			Validation data	sed	Weed Manager predictions
Oxford 1[*]	32 (sensitive)	none	6.7	0.52	6.1
		Isoproturon (late November)	7.6		6.9
Oxford 2[*]	113 (sensitive)	none	7.4	0.35	5.3
		Isoproturon (late November)	8.0		6.5
ADAS Boxworth 3[+]	144 (metabolic resistance)	none	4.9	na	6.3
		Full – [flufenacet + pendimethalin (mid October) and clodinafop + trifluralin and flupyrsulfuron (mid December)]	9.2		8.9
		Early – [flupyrsulfuron and pendimethalin (early December)]	7.1		8.0
		Late – [iodosulfuron+mesosulfuron (late January)]	8.7		8.9

[*] Wilson 1980; [+] Tatnell - unpublished data from 2004

Fig 1.

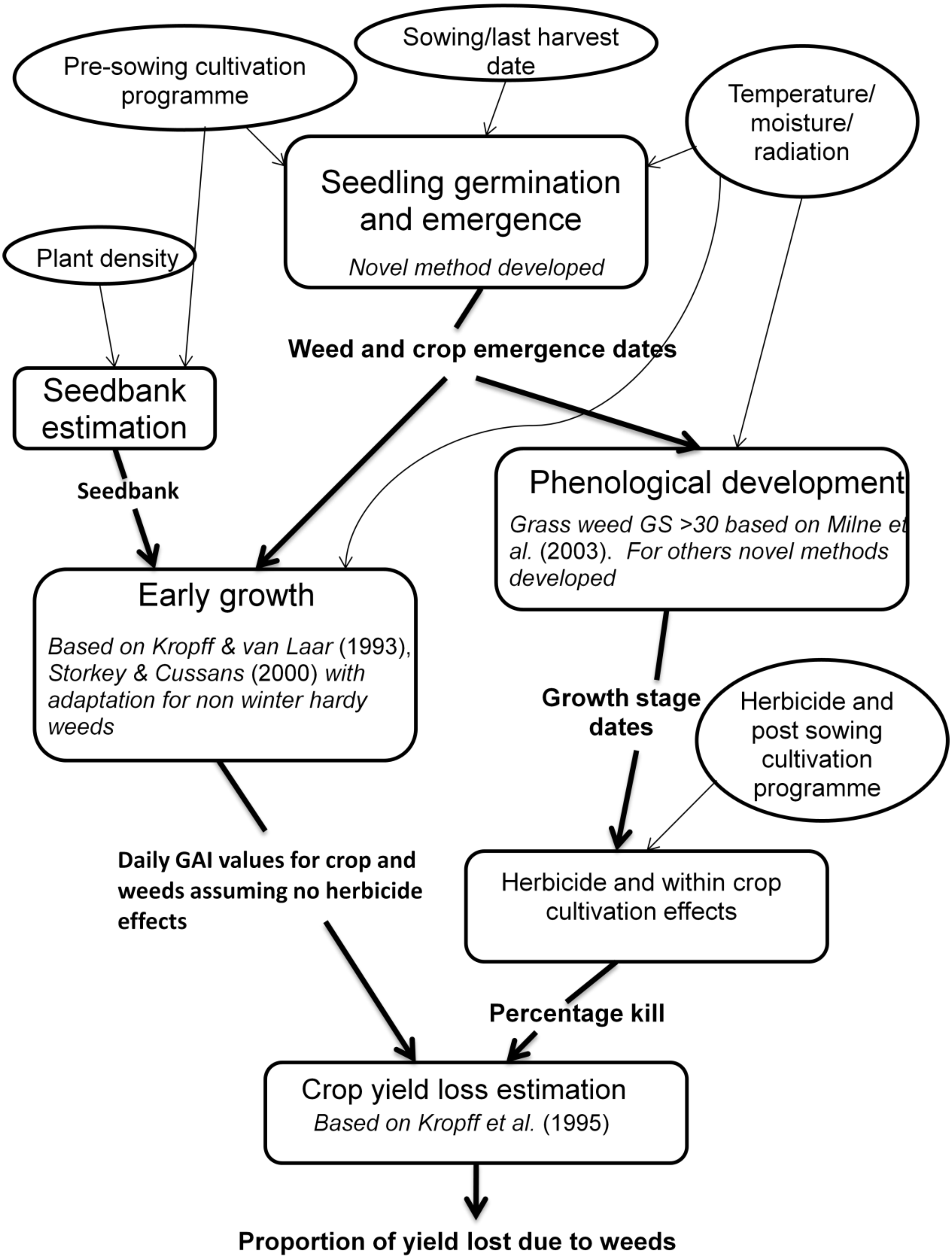
Pre-sowing cultivation programme
Sowing/last harvest date
Temperature/ moisture/ radiation
Seedling germination and emergence
Novel method developed
Plant density
Seedbank estimation
Weed and crop emergence dates
Seedbank
Phenological development
Grass weed GS >30 based on Milne et al. (2003). For others novel methods developed
Early growth
Based on Kropff & van Laar (1993), Storkey & Cussans (2000) with adaptation for non winter hardy weeds
Growth stage dates
Herbicide and post sowing cultivation programme
Daily GAI values for crop and weeds assuming no herbicide effects
Herbicide and within crop cultivation effects
Percentage kill
Crop yield loss estimation
Based on Kropff et al. (1995)
Proportion of yield lost due to weeds

Fig. 2