Analysis, Development and Application of Wheat Models of Differing Complexity at the Farm and Field Scale

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Abstract

The development and analysis of crop models of differing complexity is presented, ranging from a simple, static, empirical model, to more complex, dynamic, mechanistic models. Two models, an existing mechanistic model (Sirius) and a new mechanistic model of more intermediate complexity (Intermediate), were developed and analysed using relatively detailed field-level observations. In contrast, two new simpler models, an empirical and a mechanistic model, were developed using relatively coarse farm-level observations.

Analysis of the existing mechanistic model (Sirius) revealed that a number of model variables and cultivar-specific parameters were redundant and did not contribute to model performance. The results of this analysis informed the development of mechanistic model of more intermediate complexity (Intermediate), although this was also indicated to contain redundant variables and parameters. Vernalisation simulation was one aspect of the models that was consistently identified as an area of redundancy. These reduced models are a product of the data used to generate the reduced model – in this work, simplified versions of the models were identified that were capable of maintaining the ability to predict differences in cultivar growth and development under different nitrogen treatments. Careful consideration needs to be given to the application of the reduced model, to inform the data used in the reduction. Automated, comprehensive model reduction techniques, such as the one employed here, have the potential to be important tools in reducing unnecessary model complexity, and associated uncertainty, for an application. This unnecessary complexity can act as a barrier to application, analysis and understanding.

An empirical (Simple-EMP) and simple mechanistic (Simple-MECH) model were additionally developed to predict wheat yield at the farm-scale, using farm-level observations. The empirical model produced more accurate predictions of wheat yields than the mechanistic design, which was hindered by the monthly time step necessitated by the driving meteorological observations and the lack of traditional mechanistic model input observations. The farm-level survey data from which these models were developed is collected annually, and suggestions for further development of these models are made, including (i) incorporating newly available data on fertiliser application to replace the existing proxy, and (ii) exploring the potential to obtain additional data traditionally required by crop models, primarily the timing of important management decisions, for example, sowing and harvest dates.

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Declaration

I hereby declare that the work presented in this thesis is my own work and has not been submitted for any other degree. All sources of information have been acknowledged by reference to the authors.

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List of Abbreviations and Symbols

Abbreviation / Symbol	Definition
A_SUM	Intermediate variable used in the calculation of vapour pressure deficit, used in the calculation of evaporation
a_1	Factor describing effect of fertiliser on canopy size (1)
a_2	Factor describing effect of fertiliser on canopy size (2)
A_{fert}	Model parameter; Proportion of canopy size attributable to fertiliser and/or manure application
AGMIP	Agricultural Model Inter-comparison and Improvement Project
AHDB	Agriculture and Horticulture Development Board
ALPHA	Factor representing the effect of canopy shading on soil surface evaporation
A_M	Applied manure (kg)
A_{max}	Potential maximum leaf size (m^2)
B	Biomass (t ha^{-1})
B_d	Biomass threshold (t ha^{-1})
BIOANTH	Biomass at anthesis (t ha^{-1})
B_l	Model variable; Proportion of crop biomass lost due to rainfall damage (kg ha^{-1})
B_S	Stem biomass (kg m^{-2})
°C	Degrees Celsius
°Cd	Degree day (°Cd)
C_F	Cost of fertiliser (£ ha^{-1})
CO_2	Carbon Dioxide
CONDUC	Denominator in the correction applied to air temperature to estimate canopy temperature
CP	Crop Protection
C_S	Cost of sprays applied (£)
CV	Coefficient of variation (%)
d	Day
D	Soil profile depth (m)
DAS	Days after sowing (days)
DEFRA	Department for Environment, Food and Rural Affairs
DM	Dry matter
DP_F	Deflated index of fertiliser prices
DWP	Deflated wheat price (£)
ENAV	Variable influencing the calculation of canopy temperature and maximum soil temperature

Abbreviation / Symbol	Definition
ET	Environment Type
$EVAP_{POT}$	Water available for evaporation (mm d-1)
EW	Intermediate variable used in the calculation of vapour pressure deficit, used in the calculation of evaporation
F	Model output variable
FAO	Food and Agriculture Organisation
FAOSTAT	Food and Agriculture Organization Corporate Statistical Database
FBS	Farm Business Survey
$F_{capture}$	Fraction of plant available soil water and nitrogen that can be captured by the crop
F_D	Daylength factor
FLN	Final leaf number
F_m	Factor representing the influence of soil moisture on nitrogen mineralisation
F_v	Vernalisation factor
F_{vzero}	Un-vernalised development rate
g	Grams
GAKILR	Factor effect of drought on canopy senescence
GCM	Global Climate Model
GDD	Growing Degree Days (°Cd)
G_F	Grainfill factor
ha	Hectare
HGCA	Home Grown Cereals Authority
HI	Harvest index
HSLOP_TMEAN	Intermediate variable used in calculation of Priestly-Taylor evaporation
Intermediate	Model; intermediate complexity, field-scale
Intermediate-R	Model; reduced form of Intermediate model
K_e	Extinction coefficient
K_{fert}	Parameter describing shape of relationship between fertiliser and LAI
kg	Kilograms
km	Kilometres
kPa	Kilopascal
K_{spray}	Factor describing shape of relationship between cost of spays applied and LAI
L_{actual}	Nutrient limited increase in LAI
LAI	Leaf Area Index
LAI_0	Parameter describing canopy size - maximum in the absence of fertiliser
LAI_{int}	Canopy size
LAI_{pot}	Potential increase in LAI

Abbreviation / Symbol	Definition
LAI_{μ}	Parameter describing canopy timing
LAI_{σ}	Parameter describing canopy duration
LEAFDEMAND	Daily leaf area nitrogen demand calculation from leaf area expansion and leaf nitrogen requirements (g)
LF_{max}	Maximum possible leaf number
LF_{min}	Minimum possible leaf number
L_N	Leaf nitrogen (kg N m^{-2})
LUE	Light Use Efficiency (gMJ^{-1})
m	Metre
m^2	Square metre
$maxS_N$	Maximum stem nitrogen concentration (kg N kg^{-1} DM)
MCMC	Markov Chain Monte Carlo
MH	Metropolis-Hastings
$minS_N$	Minimum stem nitrogen concentration (kg N kg^{-1} DM)
mm	Milometers
ms^{-1}	Metres per second
N	Nitrogen (kg ha^{-1})
n	Number of observations
N_f	Ratio between plant available nitrogen and nitrogen required for potential growth
N_{tra}	Nitrogen available to the crop (kg ha^{-1})
NUE	Nitrogen Use Efficiency (kg DM kg^{-1} N)
$\bar{O}$	Mean of observed values
O_i	*i*th observation
OM	OpenModel
P	Model parameter
P_0	Baseline value of model parameter
P1D	Parameter describing photoperiod sensitivity
P1V	Parameter describing vernalisation requirement
PAR	Photo-synthetically Active Radiation
PHYLL	Phyllochron (°Cd)
P_i	Ith predicted value
POTLFNO	Potential number of leaves
PP	Daily photoperiod (hours)
PRIMORDNO	Primordia number
P_{total}	Total wheat production (t)
PTSOIL	Intermediate variable used in the calculation of soil surface evaporation
$Q_{current}$	Pseudo-likelihood of trial model prediction
Q_i	Pseudo-likelihood of a reduced model
QTL	Quantitative Trait Loci

Abbreviation / Symbol	Definition
Q_{trial}	Pseudo-likelihood of currently accepted model prediction
r	Random value
R	Rainfall (mm)
R1, R2, R3, R4	Round of estimation
r^2	r^2 statistic
r^2_{adj}	Adjusted r^2 statistic
Rad	Radiation (MJ m^{-2} $month^{-1}$)
RCM	Regional Climate Model
Rd	Rainfall threshold (mm)
RL	Root length (m)
R_p	Parameter replacement probability
RUE	Radiation Use Efficiency (gMJ^{-1})
s	Number of adjustable parameters (in the model)
S	Sensitivity
S_CTEMP	Switch to set canopy temperature to air temperature
S_HTEMP	Switch for diurnal temperature adjustment
S_SOILMAX	Switch to set the estimate of maximum soil temperature to maximum air temperature
S_SOILMIN	Switch to set the estimate of minimum soil temperature to minimum air temperature
S_VERN	Switch to remove the influence of vernalisation on crop development
s.e.	Standard Error
S_{DUL}	Drained upper limit of soil layer
SF	Factor representing the effect of drought on canopy expansion
S_f	Ratio between actual and potential evapotranspiration
Simple-EMP	Model; low complexity, empirical, farm-level (new)
Simple-MECH	Model; low complexity, mechanistic, farm-level (new)
Sirius-R	Model; high complexity, reduced version of Sirius (new)
SLDL	Daylength response
S_{LL}	Lower limit of soil layer
SLN	Specific Leaf Nitrogen (kg N m^{-2})
SLOSL	Intermediate variable used in calculation of soil surface evaporation
SLW	Specific Leaf Weight
S_N	Stem nitrogen (kg N m^{-2})
S_{SAT}	Saturation of soil layer
SS_{tot}	Total sum of squares
SW	Soil water (mm)
SW_{max}	Maximum water storage capacity of the soil (mm)

Abbreviation / Symbol	Definition
t	Time
t	Tonnes
TA	Seven-day moving average air temperature (°C)
TADJ	Temperature correction for calculation of soil temperature
T_b	Base temperature (°C)
TE	Transpiration equivalent (kg ha^{-1} mm^{-1})
T_{max}	Maximum daily temperature (°C)
T_{min}	Minimum daily temperature (°C)
T_N	Total available nitrogen (kg m^{-2})
TT	Thermal Time (°Cd)
TTANBGF	Thermal time from anthesis to the beginning of grain fill (°Cd)
TTANTH	Thermal time from emergence to anthesis (°Cd)
TTBGEG	Thermal time from the beginning of grain fill to the end of grain fill (°Cd)
TTFLIN	Thermal time from emergence to floral initiation (°Cd)
TT_{GF}	Thermal time elapsed since start of grain fill (°Cd)
TTSOWEM	Thermal time from sowing to emergence (°Cd)
V_DAYS	Daily increment in number of vernalising days (days)
VAI	Response of vernalisation rate to temperature ($°C^{-1}$)
VBEE	Vernalisation rate at 0°C (1/days)
Vdays	Accumulated vernalising days
VPROG	Vernalisation progress
W	Water in the soil profile (mm)
WF_{ratio}	Wheat-fertiliser price ratio
W_i	Weight associated with the *i*th observation
(w)MAE	(Weighted) Mean absolute error
(w)MAPE	(Weighted) Mean percentage error
(W)SS_{res} / RSS	(Weighted) residual sum of squares
WND	Wind speed (m s^{-1})
WP	Water Productivity (kg m^{-3})
WSS_{exp}	Explained sum of squares
WSSresfull	Weighted residual sums of squares for the full model
WSSresi	Weighted residual sums of squares for the *i*th reduced model
WSS_{tot}	Weighted total sum of squares
WU	Water use (mm)
WUE	Water Use Efficiency (kg m^{-3})
x	Value of parameter
Y	Yield (kg ha or g m-2)
Y_{value}	Deflated value of wheat yield (£)

Abbreviation / Symbol	Definition
α	Constant controlling how WSS_{res} affects belief in the model
μ	Mean
σ	Standard deviation

1 Introduction

1.1 Cereals in Agriculture

Cereal crops – grasses cultivated primarily for their grain – are of global importance because of their role as staple foods. Cereals have been cultivated since agriculture began c. 12,000 years ago (Tanno and Willcox, 2006). Rice, wheat and maize are the three most important food crops globally, with over 50% of calories consumed by humans derived directly from the grains of these cereals. Cereals also provide an important food source for livestock, which in turn, are a major component of human diets (Awika et al., 2011).

Since cereals were first cultivated improvements in yield have been obtained by optimisation of management and the breeding of new, higher yielding cultivated varieties (cultivars). Initially, wild landraces were cultivated, with the first domesticated varieties appearing 2,000 years later. It was not until the Agricultural, Industrial and Green Revolutions of the 18th, 19th and 20th centuries that significant increases in yield were attained (Figure 1.1). The mechanisation of agriculture and subsequent production of synthetic nitrogen-based fertilisers, together with the introduction of improved irrigation and crop rotation programs and breeding of new high-yielding semi-dwarf varieties with resistance to lodging, pests and diseases, contributed to improving crop yields (Evenson and Gollin, 2003; Moseley, 2015). Global trends in cereal production, area harvested and yield are depicted in Figure 1.2 (FAOSTAT, 2017), where production refers to the weight of the harvested product (i.e. grain), whilst yield refers to the weight of the harvested product (at a standard moisture content) per unit area of land (DEFRA, 2016; Fischer, 2015).

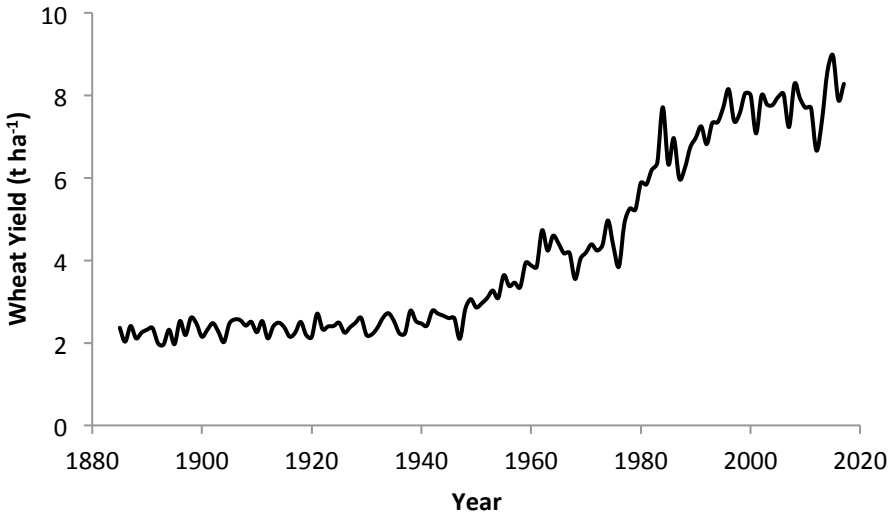


Figure 1.1 Mean United Kingdom wheat yields 1882-2015 (DEFRA, 2017). Significant increases in wheat yields have been achieved since 1882, rising from 2-3 tha^{-1} prior to 1950, to an average of 8.3 tha^{-1} in 2017.

Historically, increases in cereal production have been the result of both increases in yield and area sown. In the future, it is likely that ccompetition from human activities and an increasing focus on limiting environmental degradation will restrict the expansion of existing agricultural area. Therefore the increase in production will need to be driven by yield increase, rather than the expansion of agricultural land area (Godfray et al., 2010; Tscharntke et al., 2012). In addition, existing area is being lost due to urbanization, as well as unsustainable agricultural practices that result in desertification, salinization and soil erosion (Nellemann, 2009). These losses are predicted to be further increased by climate change (Brown & Funk, 2008), of which the long-term effects are uncertain but include:

- A general temperature increase together with an increased frequency of short periods of extreme heat, causing heat stress. Increased temperatures could

result in either an increase of decrease in yield, depending on the climate (Darwin & Kennedy, 2000; Olesen & Bindi, 2002), whilst heat stress can be detrimental to yield (Pradhan & Prasad, 2015; Prasad & Djanaguiraman, 2014).

- Changes to precipitation, including an increase in the frequency and severity of both drought and heavy rainfall. Drought stress can cause reduce yields (Saini & Westgate, 1999) and excess rainfall that results in waterlogging can also reduce plant growth through subsequent root lodging and the formation of anaerobic soil conditions (Berry & Spink, 2012; Malik et al., 2002).
- Salinization occurs as a result of unsustainable irrigation strategies employed to address water scarcity. Depending on the soil type this can reduce crop yield through decreased water availability as the soil's permanent wilting point increases, extreme pH and ion-associated toxicity, (Pessarakli et al., 1999).
- Elevated carbon dioxide levels could result in improved yields, through higher photosynthetic rates and greater water-use efficiency (Drake et al., 1997; Kimball et al., 2002).

Since the 1980s, production increases have continued despite a reduction in area harvested (Figure 1.2). It is estimated that agricultural production will need to double to meet the requirements of the predicted global population in 2050, however the current average annual yield improvements of the top three global cereal crops (maize, rice and wheat) are below the rate required to meet this target (Ray et al., 2013). The increased economic cost of fertilizers, in addition to the environmental degradation associated with their excessive application (Fageria & Baligar, 2005; Gaju et al., 2011), makes increasing production more

challenging. There has been criticism of the magnitude of this required increase in food production, as well as a reduced revised figure of 60% (e.g. Alexandratos et al., 2012; Tomlinson, 2013). Regardless, maintaining or increasing production in the future will need to address uncertain climate change effects, whilst simultaneously optimising land, nutrient and water use in the face of rising competition for and cost of these resources (Fargione et al., 2008).

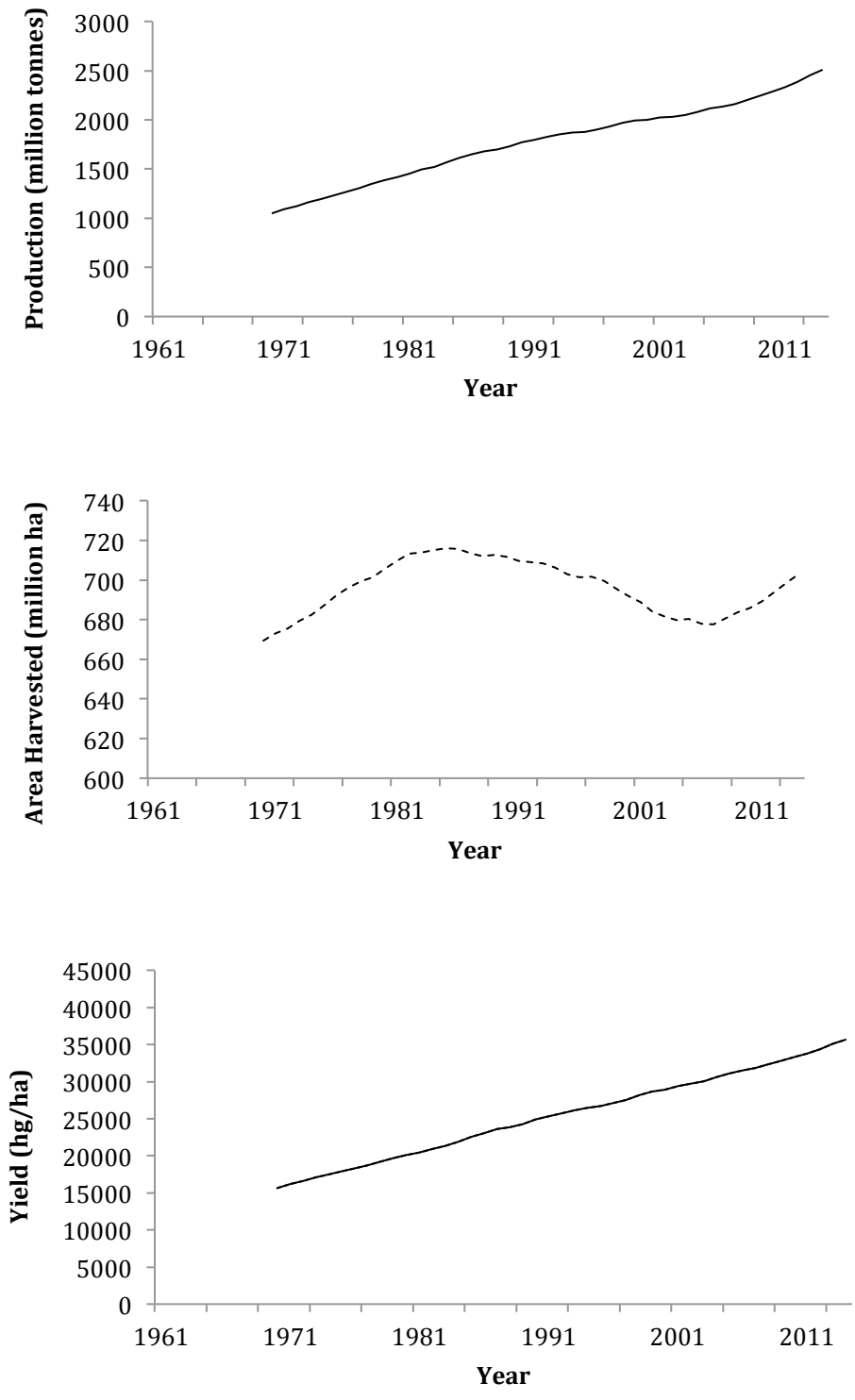


Figure 1.2 Global Total Cereal Statistics 1961-2014: (a) Production (million tonnes), (b) Area Harvested (million ha) and (c) Yield (hg/ha). Displayed as a 10-Year Moving Average. (FAOSTAT, 2017).

1.2 Wheat

Wheat (*Triticum spp.*) was one of the earliest domesticated cereals (Tanno and Willcox, 2006). Flour produced from its grain can be used to produce bread, cakes, pasta, breakfast cereals and beer. The grain is also used as animal feed, with the straw providing a construction material and bedding for livestock. Globally, wheat is the second most important calorie source, providing approximately 19% of dietary energy and contributing nearly 30% of global cereal production (Ray et al., 2013). In the UK in 2017, wheat was the most widely grown crop, being grown on 1.8 million hectares of land (DEFRA, 2017a) and producing 15.2 million tonnes of grain (DEFRA, 2017b).

In comparison to other major cereals, wheat is an adaptable crop, with varieties suitable for both temperate and tropical climates, making it the most geographically distributed source of cultivated food. Cultivars are typically classified as either winter or spring wheats, referring to the flowering response of the cultivar to low temperatures, and the associated season in which they are sown. In temperate climates, such as the UK, autumn sowing of winter wheat varieties dominates, with harvesting in late summer (AHDB, 2015). For example, in the UK, winter wheat is normally sown in September or October and harvested in August. Spring wheat can be sown in Autumn or delayed until Spring, although it usually produces lower yields than winter varieties.

1.2.1 The Wheat Lifecycle

The wheat life cycle can be defined by vegetative, reproductive and grain filling phases (Figure 1.2) (AHDB, 2015). Initially in the vegetative phase, plant growth is restricted by the size of the plant's photosynthesising canopy and nutrient-absorbing root system. In the process of photosynthesis, plants use their (predominantly leaf) canopy to intercept light and synthesise the carbohydrates necessary for growth using carbon dioxide and water. During respiration, carbohydrates are oxidised to produce energy used in plant growth and maintenance. These carbohydrates are re-distributed to actively growing sites or stored as reserves for use when photosynthesis is not sufficient to meet the energy requirements of the plant (Charles-Edwards et al., 1986).

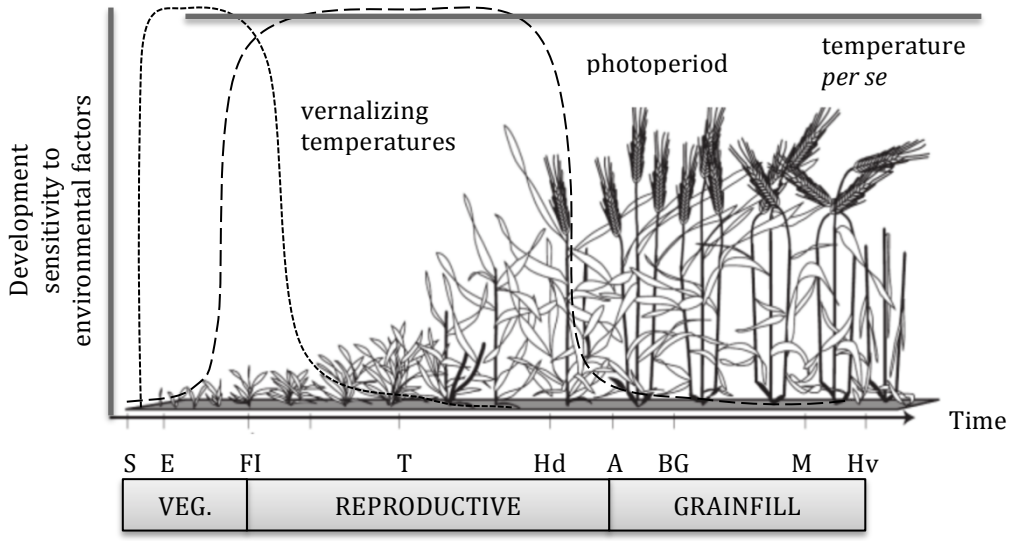


Figure 1.2 The winter wheat life cycle, as indicated by external morphology and affected by sensitivity to photoperiod and cooler temperatures. The life cycle can be divided into vegetative, reproductive and grainfill phases, defined as sowing (S) to floral initiation (FI), floral initiation to anthesis (A), and anthesis to harvest (Hv). Other key stages include emergence (E), tillering (T), heading (Hd), beginning of grain-fill (BGF) and maturity (M). Adapted from (Slafer and Rawson, 1994).

In addition to solar radiation and water, nutrients such as nitrogen, phosphorous and potassium are essential for growth. In particular, nitrogen is essential in the formation of plant structures and enzymes, as well as being a major component of chlorophyll, the pigment critical for photosynthesis (Charles-Edwards et al., 1986). Soils do not generally provide the nitrogen necessary for wheat to attain its potential yield, therefore application of nitrogen fertiliser to agricultural soils is essential. Nitrogen uptake from fertilisers is crucial in maximising canopy expansion and subsequent yield production, as a significant amount of nitrogen in leaves and stems is remobilised and redistributed to grain during grain filling (Pask et al., 2012).

In the initial phase of the wheat plan life cycle - the vegetative phase - the plant emerges and seedling growth begins, producing multiple leaves, before initiating tillering (production of lateral shoots from the base of leaves) to form a canopy (Figure 1.2)(McMaster, 2005). Following slow initial growth, the subsequent increased canopy size results in rapid growth, with the formation of deeper roots and extension of the stem (HGCA, 2008).

Floral initiation marks the transition of the plant from production of leaves to spikelets, switching from vegetative to reproductive development. With the onset of stem elongation, the jointed stalk of the wheat plant extends upwards. Stem elongation is complete when the last (flag) leaf emerges. Each stalk ends in a head, consisting of spikelets, which bear flowers and develop into grain. Shortly after flag leaf emergence, the booting stage occurs, signalling that the head is about to emerge (HGCA, 2008).

After the wheat heads, flowering (anthesis) occurs, marking the transition to grain filling. Canopy growth ceases by the time the plant flowers, with a reduction in leaf area as a result of ageing and senescence. In this final phase, grain growth occurs. Canopy death occurs before grain ripening is complete (HGCA, 2008).

The progress of a wheat plant through the stages of its lifecycle can be described using the Zadocks scale (Zadoks et al., 1974). This is a decimal code system, which is widely used to track and compare the development (or phenology) of wheat plants (Table 1.1).

Table 1.1 Key stages of Zadoks growth scale (Zadoks et al., 1974).

Decimal Code	Development Stage	Critical Management Factors
00	Sowing	Soil Preparation Pest Control
10	Emergence (Seedling Growth)	Weed Control
20	Tillering	Weed Control Nitrogen (Nutrient)
30	Stem Elongation	Nitrogen (Nutrient) Water Supply
40	Booting	Water Supply Radiation
50	Heading	Water Supply
60	Anthesis (Flowering)	Water Supply
70	Grain Filling: Milk Development	Water Supply
80	Grain Filling: Dough Development	Water Supply
90	Ripening	Pest Control

Each decimal code of the Zadock scale can be further sub-divided, for instance GS10 describes seedling growth by leaf number, increasing from GS10 (first leaf emerges), to GS11 (the first leaf has unfolded) increasing with each unfolded leaf to GS19 (signifying nine or more leaves unfolded). Important stages include; emergence (GS10), the start of stem extension (GS31), flowering (GS61), end of

grain filling (GS85) and harvest ripe (GS92). At each stage, there are different elements of management that are critical in optimising development (Table 1.1).

The development of wheat through its lifecycle is affected by temperature and other environmental factors. Its chronological progress is widely expressed in accumulated thermal time (TT), measured in Growing Degree Days (GDD, °Cd), rather than age (Equation 1.1). This allows for the variation in development, and thus the duration of the phases, due to the temperatures experienced. For wheat, GDD are usually calculated with a base temperature (T_b) of 0°C for physiological processes. This is the temperature below which no development occurs.

$$\boldsymbol{TT} = \sum[(\boldsymbol{T_{max}} + \boldsymbol{T_{min}})/\boldsymbol{2}] - \boldsymbol{T_b} \qquad \textbf{Equation 1.1}$$

Where T_{max} and T_{min} are the maximum and minimum daily temperature (°C), respectively. Each developmental stage requires a specific amount of accumulated GDD (Ruiz et al., 2016). Therefore, warmer temperatures accelerate development. However, this decrease in phase length reduces the time for growth during that phase.

Depending on the development stage, the effects of temperature can be modified slightly, with the magnitude differing with stage and variety (Rawson et al., 1998). Minor modifications include drought, nutrition and radiation, with major changes made by photoperiod (number of hours of daylight) and vernalisation (temperatures between 0 and 12°C). The vernalisation response, whereby a period of cooler temperatures during one part of the season advances flowering (anthesis), and

reduces the length of the vegetative phase in another, is strong in winter wheat varieties. Spring wheat varieties have a negligible vernalisation response, allowing them to be planted later than winter wheat varieties. Wheat varieties also differ in their response to photoperiod. Long days advance flowering, affecting both the vegetative and reproductive phases of the wheat life cycle.

Differences in photoperiod and vernalisation response, and other important physiological traits, are controlled by the genetic makeup (genotype) of a variety of which the basic unit is a gene. The physical position of a gene on a chromosome is known as its locus, with alternative forms of the same gene at the same locus being known as alleles. These alleles, in combination with the environment, determine the expression of a trait (phenotype). Examples of loci controlling photoperiod response, vernalisation requirement and plant height are listed for a number of cultivars (cultivated varieties) in Table 1.2. Depending on the allele present at the locus, a cultivar might have an increased sensitivity to photoperiod, a strong vernalisation response, and a reduced plant height, or vice versa (White & Hoogenboom, 2003). For example, the winter wheat cultivar Soissons, has low sensitivity to daylength, consistent with its photoperiod insensitive allele. It also fails to head in the absence of vernalizing temperatures, consistent with the three alleles it holds for a winter growth habit (Table 1.2; He et al., 2012).

Table 1.2 Examples of identified Loci Affecting Wheat Growth and Development. Adapted from Gaju et al, (2011), He et al. (2012). [a]Ppd-D1a allele confers insensitivity to photoperiod, whilst Ppd-D1b confers sensitivity (Gaju et al., 2011). [b]Vrn-B1d (deleted) confers a spring growth habit, while Vrn-B1nd (non-deleted) confers a winter growth habit (Fu et al., 2005). The alleles a and b confer a spring growth habit, while the allele c confers a winter growth habit (He et al., 2012; Yan et al., 2004). All cultivars were also characterised as also have the allele conferring winter growth habit at the Vrn-D1 locus (Fu et al., 2005). [c]The Rht-B1b and Rht-D1b alleles confer semi-dwarf stature (Gaju et al., 2011).

Cultivar	Photoperiod Response[a]	Vernalisation Requirement[b]		Plant Height[c]	
Arche	Ppd-D1b	Vrn-A1b	Vrn-B1nd	Rh1-B1a	Rht-D1a
Beaver	Ppd-D1b	Vrn-A1c	Vrn-B1nd	Rh1-B1a	Rht-D1b
CF9107	Ppd-D1b	Vrn-A1c	Vrn-B1d	Rh1-B1a	Rht-D1b
Paragon	Ppd-D1b	Vrn-A1a	Vrn-B1nd	Rh1-B1a	Rht-D1a
Recital	Ppd-D1a	Vrn-A1c	Vrn-B1nd	Rh1-B1b	Rht-D1a
Soissons	Ppd-D1a	Vrn-A1c	Vrn-B1nd	Rh1-B1b	Rht-D1a
Toisondor	Ppd-D1a	Vrn-A1c	Vrn-B1nd	Rh1-B1a	Rht-D1b

1.2.2 Current Challenges

The challenges facing wheat production are common to agriculture globally and outlined in Section 1.1. It is likely that the production increases required by the projected future population will be obtained by enhancing yields whilst improving

resource use efficiency, rather than the expansion of agricultural areas (Godfray et al., 2010; Ray et al., 2013; Tscharntke et al., 2012). The current rate of increase in wheat yields, however, is not sufficient to meet projected future demand (Grassini et al., 2013). As wheat is grown in a great range of climatic and geographic regions, it will therefore be subject to a great range of climate change effects. Therefore, achieving this production target will be dependent on not only the optimisation of management to maximise yields, but also the breeding of new cultivars which are capable of producing these yields under the predicted increased temperatures, changes in precipitation frequency and severity, soil salinization and increased CO_2 levels (Grassini et al., 2013; Parry & Hawkesford, 2010).

Historically, plant breeders have focused solely on maximising yield. However, they now face the challenge of developing high-yielding cultivars with increased nitrogen and water use efficiency, as well as improved stress adaptation for climatic conditions that are either uncommon or might not yet exist (Shiferaw et al., 2013). Traditionally, the breeding of new cultivars with specific adaptations has taken 10-30 years (Semenov & Halford, 2009; Chapman et al., 2012). There is the potential to improve the efficiency of the breeding process, as well as exploring and identifying solutions to the above challenges, though the application of crop models (Boote et al., 1996; Chapman et al., 2012).

1.3 Crop Models

The use of mathematical models to simulate systems was pioneered by engineers in the 1950s, and has since been adopted by a wide range of disciplines. Models are typically a simplified representation of systems, which are simulated either at a fixed

point (static), or over time (dynamic) (de Vries and van Laar, 1982). This allows the study and analysis of this system's behaviour (Yin and Struik, 2010). For example, a crop modeller could be interested in the final yield of a crop at the end of the season (static), or the production of that yield over the season (dynamic). The aim of such models is to increase knowledge of, and provide practical solutions to issues in, agricultural systems (Thornley and Johnson, 1990).

Approaches to modelling crops range from simple, empirical models (e.g. Landau et al, 2000), to more detailed, mechanistic models (e.g. Lawless et al., 2005). Empirical or statistical models describe crop growth and development, by forming relationships between observations using regression equations. Mechanistic or process-based models attempt to explain crop growth and development, by summarising current understanding of the underlying processes in the form of suitable mathematical equations. The terms 'empirical' and 'mechanistic' will be used subsequently in this thesis to distinguish to these model types.

An example of an empirical model is provided by Landau et al. (1998) who used a linear regression model to describe the final wheat yield as function of certain growth season weather effects, requiring only climatic inputs to be specified. An example of a mechanistic crop model can be demonstrated by the Sirius model (Lawless et al., 2005). A feature of dynamic, mechanistic crop models is a high degree of interaction and feedback between different components of the model. The Sirius model simulates crop growth and yield formation over time, as a function of the incident radiation and the size of the crop canopy, as potentially limited by nitrogen and water. Thus, Sirius explains the yield produced over time using interception of

radiation by the canopy, the growth of which can be restricted if sufficient nitrogen and water are not available for uptake. As well as inputs describing the climate and management decisions, mechanistic models like Sirius require additional values to be specified (i.e. parameters), for instance to describe soil characteristics and cultivar differences. Such crop models are developed in conjunction with laboratory and field experiments, literature searches and numerous model evaluations (de Vries and van Laar, 1982).

Modelling plant growth and development requires the consideration of many factors that encompass numerous fields of study. For instance, weather (meteorology), photosynthesis, respiration and transpiration (biochemistry), soil water and nutrients (soil chemistry, microbiology and physics), plant inter-competition (plant ecology) and diseases and pests (population dynamics) (de Vries and van Laar, 1982). These models are therefore often constructed out of numerous sub-models, each describing different parts of the system.

Early crop models were designed to be programmed on a pocket calculator, but quickly progressed to being programmed on computer systems (Keulen and Wolf, 1986). Most models are run on a daily time-step, but some models include processes that necessitate modelling on a shorter time-step, if the alteration of rate of change is too rapid (de Vries and van Laar, 1982). For example, the model APSIM includes soil temperature descriptions that are simulated at half hourly intervals (Holzworth et al., 2014; Keating et al., 2003). The level of model detail should be dependent on the aim of the model being developed. At the point, or field, scale, models are concerned with more detailed aspects of a crops growth and

development, whilst at the larger scale predictions are primarily focused on yield (as affected by climate change) and simulation of, for instance leaf development over time, is not necessary (Challinor et al., 2004).

Typically, dynamic crop models describe crop growth and development over the season as a function of environmental, varietal and management factors. For instance, the Sirius model requires inputs that characterise environmental conditions and management decisions in order to produce predictions of leaf area, biomass and yield (Jamieson & Semenov, 2000). The phenology of the crop is also simulated, with a focus on important developmental stages, such as emergence and anthesis date.

Explaining plant growth and development at the crop or whole plant level using physiological explanations is challenging. Although crop yield can be expressed as a function of management factors, the responses of that yield to those management decisions is a result of underlying physiology (Goudriaan and Van Laar, 2012). Therefore, whilst primarily, agronomists are interested in the whole plant, and the effect of their environment upon their growth and development, extensive research has been performed to identify biochemical and physical processes responsible for these effects. For example, the crop can be split into individual plants, then to organs (e.g. stem, root, leaf, grain), tissues (e.g. epidermis), cells, the organelles (e.g. chloroplast) and molecules (e.g. proteins) (Charles-Edwards et al., 1986).

There are numerous mechanistic simulation models of wheat, with 27 models named in the agricultural model improvement and inter-comparison project – AGMIP (Asseng et al., 2013). These adopt a variety of approaches to processes such as

canopy formation, evapotranspiration and light utilisation. For example, in cereals, the increase in canopy size as a result of increased leaf number and area is supplemented by tillering. However, when simulating canopy formation, some models explicitly simulate tiller production (e.g. CERES), whilst others describe individual leaf development (e.g. Sirius) and others simply canopy cover as a whole (e.g. Aquacrop; Studeto et al., 2009).

Models represent decades of crop research. They have been constructed to include representations of important processes controlling wheat growth and development. Mechanistic crop models therefore focus on the processes of carbon, water and nitrogen balance, with temperature, drought and nitrogen availability affecting growth and development. A few models consider other nutrient elements, most commonly phosphorous (e.g. APSIM), which is the second major growth-limiting nutrient after nitrogen in agricultural soils (Schachtman et al., 1998).

Mechanistic crop models are usually based on simulation of growth through interception and conversion of radiation into biomass and canopy expansion (Monteith, 1977). The efficiency of conversion of this radiation by a crop is usually termed Radiation Use Efficiency (RUE), with the interception of this radiation by the canopy described by an extinction coefficient (K_e) (e.g. Sirius, CERES)(de Vries and van Laar, 1982). An alternative to this RUE approach is Water Use Efficiency (WUE). In which growth is water-driven and transpiration is calculated first, with biomass then determined from Water Productivity (WP) (e.g. Aquacrop; Hsaio et al., 2009; Raes et al., 2009; Steduto et al., 2009).

Growth in biomass is usually allocated to crop roots, leaves, stem and grain according to developmental stage, growing at a potential rate or towards a potential maximum biomass or area, subject to limitation by non-optimal water, temperature and nitrogen. Nitrogen and water limitation are usually determined using simple factors, comparing demand and availability. Soil water and nitrogen availability are considered similarly, as the availability of soil nitrogen is analogous to water (de Vries and van Laar, 1982). After uptake however, within the plant, unlike water, all nitrogen is not mobile, as it is utilised in constructing plant structures (Ma et al., 2008).

Whilst most models operate at the field scale (e.g. APSIM, CropSyst), some are designed for use at the regional scale (e.g. GLAM, WOFOST). Of the 27 wheat models included in the study performed by Asseng et al. (2013), 23 were listed as primarily being field scale models. Some examples of crop models and their main features are listed in Table 1.3. The number of parameters required by these models to describe differences between wheat cultivars ranges from 2 to 22. Many of the models are descended from the same earlier model. For instance, of the 27 wheat models included in the study performed by Asseng et al. (2013), 12 are descended from just two earlier models, CERES and SUCROS.

The classification of crop models as empirical or mechanistic is broad. A truly empirical model is a statistical one, formed of, for instance, one or more regression equation(s). However, mechanistic models ultimately contain empirical descriptions, focusing on certain crop system processes in detail, and utilising empirical descriptions to describe other (sub-) processes (Keating et al., 2018). For example,

the mechanistic crop model Sirius uses empirical descriptions for vernalisation, rather describing the underlying bio-chemical processes.

The broad nature of crop model classification can be illustrated by the GLAM model, which has been described as both a mechanistic and a hybrid model (i.e. containing a mixture of empirical and mechanistic approaches) (Di Paola et al., 2016; Watson et al., 2015). As a result of its focus on the impact of climate on yield and the regional scale at which it was designed to operate, GLAM favours simpler descriptions of processes it does consider (e.g. leaf area and yield formation) and also replaces explicit modelling of many non-climatic yield-determining processes (e.g. nitrogen fertilisation) with a single yield-gap parameter.

Although complexity is linked to model type - mechanistic models are generally more complex than empirical models - it is possible that an empirical model describing many processes could be more complex than a mechanistic model that focuses on a single, or limited number of processes. Although there is no set classification of model complexity, it can be assessed according to the number of modelled processes, the number of equations used to model those processes, or number of model parameters (Soltani & Sinclair, 2015, Di Paolo et al., 2016), in particular the number of parameters describing cultivar differences (e.g. Challinor et al., 2014). Mechanistic models generally describe more aspects of crop systems, as well as representing the underlying processes driving these aspects, utilising adjustable parameters, resulting in a more complex model.

Criticism has been levelled over the lack of clarity of the model parameters that arise in complex mechanistic models (Soltani & Sinclair, 2015; Di Paolo et al., 2016). The

number of these adjustable parameters is subjective, as well as dependent on model application. For the mechanistic model APSIM, which has a total of 292 parameters, the user is only expected to modify approximately 10% of these to simulate a given soil and crop (Soltani & Sinclair, 2015). With regard to parameters describing cultivar differences, significant differences emerge in the literature in the number considered. For example, 7 (Di Paolo et al., 2016) or 15 (Soltani & Sinclair, 2015) parameters have been considered to describe differences in wheat cultivars. Of the 211 parameters in the DSSAT crop model, there are seven parameters considered specific to individual cultivars, but a further 32 parameters describing differences in groups of cultivars (Soltani & Sinclair, 2015). Parameters that might not be declared as adjustable or cultivar-specific parameters by the authors could also be modified. For example, a parameter describing the effects of CO_2 concentration on plant growth would not normally be modified for a short-term prediction, but would become important in long-term simulations. Therefore, when considering model complexity, it is important to not just consider the number of model parameters, but also the number of processes, and the detail in which those processes are considered.

There is debate about the level of complexity that is appropriate for crop models (White et al., 2011). Ultimately the model should be selected according to the requirements of the application, which should not just be based upon a comparison of the simulation with observations (Asseng et al., 2013; Soltani & Sinclair, 2012). A large number of parameters and/or a lack of clear documentation and explanation regarding the use of parameters in model application can be a barrier to appropriate model use (Soltani & Sinclair, 2012).

Table 1.2 Examples of wheat crop simulation models. *indicates a model which is also capable of simulating other crops. **as classified by Di Paola et al., 2016. ***as reported by Asseng et al., 2013. Adapted from Di Paola et al., 2016 and Asseng et al., 2013.

Model Name	Type **	Scale	Timestep	No. of Cultivar Parameters***	Sub-Models	Reference
APSIM*	Mechanistic	Field	Daily	7	Water Nitrogen Carbon	(Keating et al., 2003)
Aquacrop*	Empirical	Field	Daily	2	Water	(Steduto et al., 2009)
CERES	Hybrid	Field	Daily	7	Water Nitrogen	(Ritchie and Otter, 1985)
CROPSYST*	Mechanistic	Field	Daily	16	Water Nitrogen	(Stöckle et al., 2003)
GLAM*	Hybrid	Regional	Daily	22	Water	(Challinor et al., 2004)
SIRIUS	Mechanistic	Field	Daily	14	Water Nitrogen	(Jamieson and Semenov, 2000)

1.3.1 The Sirius Model

Sirius is a typical example of a mechanistic crop model, simulating wheat growth and development on a daily time-step (Figure 1.5). Potential crop growth is estimated from photo-synthetically active radiation (PAR) intercepted by the crop canopy. Nitrogen and water limitations are applied to this potential biomass production using simple limitation rules. Prior to grain-filling, biomass is used to construct first leaf, and then stem biomass. All biomass production is assigned to grain growth during the grain-filling period.

Crop development is simulated using the effect of temperature, including vernalising temperatures, and daylength on crop leaf number. Leaf emergence is controlled by the phyllochron (PHYLL), one of four cultivar-specific constant thermal time parameters describing development. Final leaf number is estimated as a function of

the vernalisation and daylength experienced by the crop during growth, with the effect of these processes described by additional cultivar-specific parameters. Anthesis occurs three phyllochrons after crop leaf number reaches final leaf number.

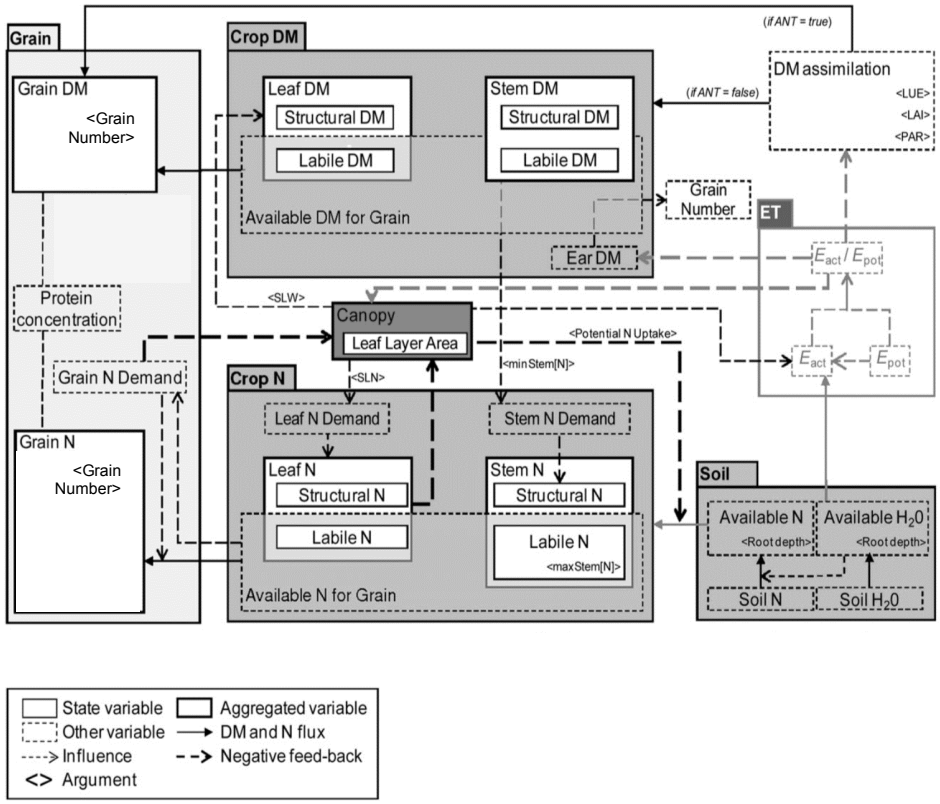


Figure 1.5 A Simplified Schematic of the Sirius Model. The main variables, influences and feedbacks are shown. ANT, anthesis; DM, dry matter; N, nitrogen; Eact, actual evapotranspiration; Epot, potential evapotranspiration; ET, evapotranspiration; LAI, leaf area index; LUE, light use efficiency; maxStem[N], maximum stem nitrogen concentration; minStemn[N], minimum stem nitrogen concentration; PAR, photosynthetically active radiation; SLN, specific leaf nitrogen (leaf nitrogen mass per unit of leaf surface area); SLW, specific leaf weight (leaf dry mass per unit of leaf surface area (Martre et al., 2006).

In total, Sirius contains 11 cultivar-specific parameters to describe differences in cultivar total biomass, grain yield, leaf area index (LAI) and anthesis date. These are summarised in Table 1.5. In addition to the cultivar-specific parameters describing thermal time durations, vernalisation and daylength, there are parameters to

describe canopy characteristics. Detailed descriptions of the model have been published (Jamieson and Semenov, 2000; Jamieson et al., 1998a; Lawless et al., 2005). The model is the subject of active development, with more recent versions focusing on detailed descriptions of crop nitrogen dynamics (Table 1.4).

It is currently one of the wheat models involved in the international AGricultural Model Improvement and Inter-comparison (AGMIP) project, applied to assess the impacts of climate change (Asseng et al., 2013; Asseng et al., 2015; Martre et al., 2015).

In terms of the models listed in Table 1.2, Sirius can be considered an intermediately complex, mechanistic model. Of the models developed at the field scale, it is more complex than Aquacrop, with its consideration of nitrogen-limited growth, in addition to water-limited growth, and explicit modelling of individual leaves rather than whole canopy cover. It is however, considerably less complex than the mechanistic model, APSIM, which utilises sub-daily descriptions, is capable of also considering phosphorous-limited growth, and also contains a carbon sub-model.

Table 1.4 Development of the Sirius Model

Model	Description	Reference
Sirius	Growth Assimilate partitioning Evapotranspiration Phenology Water-limited growth	(Jamieson & Wilson, 1988; Jamieson et al., 1989)
Sirius2000	Updated with: • Nitrogen-limited growth • Mechanistic phenology – with primordium and leaf production and final mainstem leaf number • Empirical LAI	(Jamieson et al., 1998)
Sirius2005	Updated with: • Canopy describing individual leaf and canopy layer development	(Lawless et al., 2005)
Sirius2010	Updated with: • Inter-plant competition	(Stratonovitch et al., 2012)
SiriusQuality1	Updated with: • Detailed grain protein	(Martre et al., 2006)
SiriusQuality2	Updated with: • Vertical distribution of specific leaf nitrogen in canopy	(Martre et al., 2008)

1.3.2 Current Applications

Crop models have the potential to be important tools in exploring and identifying solutions to the challenges facing wheat (Yin and Struik, 2010), which were previously outlined in Section 1.2.2. A dynamic crop model can provide analysis of crop growth and development over time, providing recommendations for optimal management, as well as increasing understanding of underlying mechanisms and processes.

Crop models can be applied to predict the optimum sowing date and density (Andarzian et al., 2015), cultivar (e.g. Stratonovitch & Semenov, 2014; Zheng et al., 2013), timing and quantity of fertiliser applications (e.g. Baret et al., 2007) and irrigation (e.g. Tubiello et al., 2000) for a specific soil type and climate by simulating the effect of these management decisions on crop growth and phenology (Manzanares et al., 1997; Singh et al., 2008). Depending on the stakeholder, this optimum may differ. For example, a researcher may be interested in attaining the highest yield, whilst a farmer may be aiming for the greatest profit (yield per unit fertiliser), for the coming year or to ensure that policies concerning fertiliser application quantity and water quality are adhered to (Lobell et al., 2009; Ewert et al., 2011).

Application of crop models can also provide insight. For example, a crop model can be applied to investigate a combination of traits, or complex traits, for example nitrogen and water use efficiency, through alteration of model parameters that can be linked to physiological traits (Foulkes et al., 2007; Semenov et al., 2009; Hammer et al., 2010). Alteration of parameters describing cultivar differences within a model

allows simulation of a hypothetical cultivar, or a number of cultivars, over numerous different environments (Semenov et al., 2014).

In an investigation into wheat traits controlling nitrogen use efficiency (NUE, grain yield per unit available soil nitrogen), a number of parameters of the Sirius model, which represented relevant traits, were altered to assess their impact (Semenov et al., 2007). A reduction in one of the parameters, controlling the specific leaf nitrogen, was demonstrated to increase NUE across all cultivars, sites, and nitrogen treatments, indicating the potential of this trait as a method for yield improvement that could be targeted through breeding (Semenov et al., 2007). Similarly, the same model was applied to assess the potential for yield improvement in water-limited conditions (Semenov et al., 2009). Results from this simulation indicated that phenology, as assessed by modifying parameters describing the phyllochron and duration of grain fill, was already optimised for the climates considered, as the alteration of these parameters did not improve yields.

In another example, the APSIM model was applied to simulate differences in height between genotypes of Sorghum (Hammer et al., 2010). Experimental observations demonstrated a genetic link between height, biomass partitioning and radiation use efficiency. When these observed relationships were incorporated into the model, increased leaf senescence as a result of greater nitrogen remobilisation was simulated in the taller genotypes. This suggested a link between the height phenotype and senescent phenotype, an effect supported by earlier experimental observations (van Oosterom et al., 2010).

The same model was applied to investigate potential traits for drought adaptation in Sorghum in India (Kholova et al., 2014). The model indicated that traits associated with leaf development could improve grain yield under severe drought conditions. However, it also simulated that the traits identified as beneficial under severe conditions, resulted in a loss of stomer (leaves and stalks) under milder conditions (Kholova et al., 2014). Stomer has an economic value as fodder, and this application demonstrates the potential of crop models to consider the impact of trait modification at the whole plant-level, rather than assessing its benefit or detriment to a sole target trait (Kholova et al., 2014).

Similarly to the above examples, crop models can be applied to explain interpret the results of plant breeding trials (e.g. Chapman, 2008). To assist plant breeding programmes, crop models can be applied to perform simulations over the long-term at multiple locations, characterising the environment types (ETs) that a crop will likely experience (e.g. Chenu et al., 2011). Using historical weather data, crop models can characterise, for instance, different drought ETs and how they are affected by rainfall, soil type and temperature (Chapman et al., 2012). Rather than the more 'static' assessment of traditional field trials, with a restricted number of experimental setups for the cultivars and environments of interest, crop models offer the potential to provide a more complete and dynamic assessment – exploring numerous traits and ETs and generating a summary of the relationship between these traits and yield across the ETs (Messina et al., 2011). These 'yield-trait performance maps' can aid in understanding the interaction between genotype and environment (Chapman et al., 2012). Information generated by such applications can then be used to design experiments or select trial locations within breeding programs to focus on the most

frequently experienced ETs and the traits that perform well under those environmental conditions (Chenu et al., 2013). The potential for crop models to assist in plant breeding programmes has been slowed however, by adaptation trade-offs. For instance, a cultivar that has increased transpiration and leaf growth under drought can deplete available soil water and as a result produce reduced yields (Chenu et al., 2009). The potential of crop models to contribute further to plant breeding programs, by simulate cultivar differences through integrating the underlying genetic information is discussed further in Section 1.3.2.1.

In the above described applications, crop models have the potential to improve the efficiency of the plant breeding process, as well as reducing the associated time and costs required, by decomposing complex traits, allowing experimental work to focus on traits with the greatest potential, and by reducing the amount of sites and seasons that are necessary for field evaluation of a new cultivar (Boote et al., 1996; Chenu et al., 2013; Messina et al., 2011). Additionally, crop models can be applied to answer research questions that cannot be practically experimentally investigated, for instance estimating deep drainage across a range of agricultural soils (Asseng et al., 2001).

Crop models can be applied to identify ‘climate-smart agriculture’, that is agriculture that sustainably increases yield, through resilience to climate change and reduction in greenhouse gas emissions (Wheeler & von Braun, 2013). Climate-smart agriculture practices can include conservation agriculture and use of improved seeds. For example, empirical models were developed to assess the effect of adaptation options on the maize yields of Zambian smallholders (Arslan et al., 2015)

taking account of socio-economic and climatic factors. The analysis identified only one of three potential forms of conservation agriculture – legume intercropping – as beneficial, with a yield increase seen even under temperature and rainfall stresses during the growing season. The benefits of fertiliser application and use of improved seeds to yield were reduced or negated by these climatic stresses. Rather, prompt access to fertiliser was important in maximising yield (Arslan et al., 2015).

In another example, the APSIM model was applied to assess mitigation options for nitrous oxide (N_2O) - a key greenhouse gas associated with climate change. If land use is changed from pasture to crop, there is an associated release of N_2O. The model was applied to identify opportunities to mitigate these emissions whilst maximising yield, through optimising the time of conversion from pasture to crop and subsequent nitrogen management (Mielenz et al., 2017). The predictions indicated reducing the length of the fallow period (between pasture conversion and sowing) would reduce N_2O emission by more than half in the first year, without reducing yield. Additionally, in this first year, the nitrogen requirement of the crop could be fully met by soil nitrogen, i.e. no nitrogen fertiliser was required. Thus, the model provided recommendations on how to reduce expenditure, whilst mitigating emissions of an important greenhouse gas (Mielenz et al., 2017).

In addition to simulating grain yield, a number of modern crop models are also capable of simulating the quality of the grain, by considering grain nitrogen and protein content (e.g. Sirius-Quality; Matre et al., 2006, APSIM; Asseng & Milroy; 2006), which allows the nutritional value of the yield to be determined (Nuttall et al., 2017). This is potentially important for the development of models as tools of

genuine value to farmers as grain quality is difficult to manage and an important element of price premium.

The APSIM model provides a further demonstration of the direct farm-level use of models, providing risk assessments for Australian farms, as part of a web application known as Yield Prophet (Hochman et al., 2009). This subscription service provides real-time information to farmers, who can assess the impact of climate alongside management strategies on their wheat crop. This service is utilised most heavily during months when nitrogen fertiliser application is determined (Hochman et al., 2009).

Crop models can also be incorporated into frameworks, to allow consideration of environmental, social and economic factors. For example, the crop model APES has been incorporated into the assessment framework SEAMLESS, alongside models describing environmental, social and economic factors (van Ittersum et al., 2008). This allows the impact of policy scenarios on cropping systems (e.g. maize, wheat, soyabean), economic (e.g. farm income) and environmental (e.g. nitrate leaching, soil organic matter) indicators on farms to be assessed within the European Union at field, farm and market level (Uthes et al., 2010).

In considering the challenges facing agriculture, current crop modelling research has focused on; (i) adapting and developing new models for modelling at the genetic level and (ii) adapting current and developing new models for modelling at the larger-than-field scale (Hammer et al., 2010).

1.3.2.1 The Genetic Level

One aspect of crop models that has been identified as requiring improvement is their ability to simulate cultivar differences. Incorporating genomic information into crop models has been suggested as one method to address this. Traditionally, parameters that represent cultivar differences are determined empirically through calibration of phenotypic experimental data, which can produce parameters that have little biological meaning (White, 2006; Yin and Struik, 2010). This limits the ability of the model to accurately simulate the wide range of plant responses to environmental, management and genetic factors (Bertin et al., 2010). Therefore, although crop simulation models are currently able to predict the effects of environment and management on crop growth and development, their ability to accurately simulate differences in cultivars is poor (Bannayan et al., 2007). Whilst crop models have been shown to explain yield differences of a genotype among highly different environments (Kropff et al., 1994), the challenge is to predict differences in performance of relatively similar genotypes (Yin and Struik, 2010). Improving this accuracy is particularly important when model application involves more complex situations, such as the assessment of the effect of climate change on crop growth processes when considering the variable nature of soil, climate and management practices (Bannayan et al., 2007).

Initial attempts have been made by linking specific genes, or regions of the genome (Quantitative Trait Loci – QTL), with physiological traits or processes, which in turn are linked back to model parameters (Tardieu, 2003; Yin and Struik, 2008). This is known as gene- or QTL- based modelling. This is challenging, as the expression of a crop's genes (phenotype) can be regulated by multiple, interacting genes, as well

its environment (Yin and Struik, 2010). Although numerous plant genes and their functions have been identified, to provide value in crop models it is necessary to identify those genes that are important in producing desirable agricultural phenotypes (White and Hoogenboom, 1996). Existing models can then be modified to replace empirical cultivar parameters with parameters estimated as a function of the alleles present at known loci (Bannayan et al., 2007). Development of such a model requires the selected genes to be identified in a large germplasm that is known to vary for the genes of interest. The calibration of cultivar coefficients is performed using this data through the traditional approach of optimising the agreement between observed and simulated data through parameter adjustment.

This approach was pioneered by White and Hoogenboom (1996), with the development of the GeneGro model, which was derived from the BEANGRO crop simulation model, developed for the dry bean (*Phaseolus vulgaris L.*) The effects of seven genes affecting phenology, growth habit and seed size were incorporated, replacing the empirically derived cultivar-specific coefficients of BEANGRO with coefficients calculated from genomic information, to produce the GeneGro model (White and Hoogenboom, 2003). This research demonstrated that it was possible to successfully incorporate genetic information into existing crop models, with the resulting gene-based model able to successfully simulate genotypes in new environments (White, 2006). An additional benefit was the reduction in the number of coefficients required to describe cultivar differences from 21 to 7, with values for these coefficients able to be determined without field calibration data. Further research performed by the same authors however, demonstrated that this approach could be limited by a lack of genetic characterisation of cultivars for genes

considered and a lack of data from environments where phenotypic differences in a gene would be expected (Hoogenboom and White, 2003). The development of GeneGro not only demonstrated the potential for genomic integration into existing crop simulation models, but also illustrated that a small number of genes could potentially account for a large amount of variation in crop phenology (Bannayan et al., 2007; White and Hoogenboom, 1996).

White (2009) argues that small numbers of genes can be used successfully in this way as simplifications to the genomic 'system' are possible. For instance, many genes may mainly affect disease or pest resistance, therefore they would have little direct effect on processes utilised to predict phenotype in current crop models. Further, complex processes such as pollination and fertilisation may have limited relevance, alongside cell division and signalling systems (Kaplan, 2001).

Since GeneGro, further gene-based models have been developed, for example a model of heading time for wheat was developed using the effects of the main photoperiod (Ppd-D1) and vernalisation (Vrn1) genes (Zheng et al., 2013). There is, however, an alternative approach that employs a higher-level of gene representation. Identification of individual major genes for physiological traits is still challenging, as a result of many quantitative traits in crops being regulated by polygenes. This restricts the progress of gene-based modelling (Bannayan et al., 2007; White, 2006), therefore, the majority of research investigating the integration of genomics into crop models uses this 'higher-level' of representation in the form of Quantitative Trait Loci (QTL) (Quilot et al., 2005; Yin et al., 2004). QTL are regions of the genome associated with trait differences (Maloof, 2003), which can be mapped using

molecular markers to identify desirable QTL alleles that can be selected for crop improvement (Yin and Struik, 2010; Yin et al., 1999). In QTL analyses, statistical methods are used to determine loci with the strongest association with the parameter, these being the QTL (White, 2006). QTLs are then incorporated into crop models similar to the gene-based approach described above (White and Hoogenboom, 1996).

As a result of their potential in describing cultivar differences in crop models, research aiming to identifying QTLs for specific crop traits is increasing. Identification of QTLs for flowering time is an especially important focus for research, as understanding this process is important for maximising crop productivity through management and breeding (Bannayan et al., 2007). For instance, QTLs for the flowering dates of rice and barley (Nakagawa et al., 2005; Yin et al., 2005) and the heading date of rice and barley (Emebiri and Moody, 2006; Liu et al., 2007) have been determined. QTLs for fatty acid content in rapeseed (Zhang et al., 2008) and wheat grain (Wang et al., 2011), as well as those for protein and oil contents of Soybean seeds (Liang et al., 2010) have also been identified. Leaf-related QTLs, such as those for leaf emergence rate (Dong et al., 2004), ratio of Rubisco to total leaf nitrogen (Ishimaru et al., 2001) and leaf rolling have been determined in rice (Price et al., 1997), as well as that for maximum root length (Price and Tomos, 1997). QTLs for plant and ear height have also been determined for maize (Zhang et al., 2010).

When considering the genetic basis for more complex plant traits that have multiple contributing genes, such as yield, it has been suggested that these should be

considered in components, for example grain weight or grains per spike (Slafer et al., 1996). For wheat grain yield, numerous QTL on different chromosomes have been identified (Curtis & Halford, 2014). Although some QTL for yield variation were determined for European winter wheat over multiple sites and seasons, others were specific to one site or season (Snape et al., 2007). In this instance, the genes or QTLs for these components can be investigated instead, rather than yield directly (Backes et al., 1995; Zhou et al., 2001). Research has identified QTLs for yield components in numerous crops, for example spikelets per plant in rice (Kato, 2004), seed size in rice (Ishimaru, 2003) and wheat (Breseghello and Sorrells, 2007) and boll weight in cotton (Zhang et al., 2011).

When considering the QTL-based approach of genomic integration, the major limitation to the utilisation of QTLs in crop simulation models is their instability across environmental conditions. QTL can alter in number and location under changing environmental conditions and developmental stages (Quilot et al., 2005; Yin and Struik, 2010; Hirel et al., 2001). Therefore, QTL analysis cannot be utilised to predict the behaviour of a genotype for an environment that is different to that in which the QTL was detected. Thus, it has been suggested that their application in modelling is appropriate prior to identification of the associated gene. Unless a stable QTL for the trait can be identified, once the gene-base for the quantitative trait has been determined, this can replace the QTL information in the model (Bannayan et al., 2007).

Yin & Struik (2010) noted that currently QTL-based models usually produced predictions nearly comparable to that of the original parameters, with any gain in

accuracy attained from the removal of random noise in the original parameters was approximately lost due to reduced accuracy as a result of identified QTLs not accounting for 100% of the genetic variance of the parameter values, e.g. (Yin et al., 2005). Focusing on identifying additional relevant QTLs to account for a greater proportion of this variance could improve this accuracy further.

Gene- and QTL-based modelling have been demonstrated to be successful in initial attempts (e.g. Chenu et al., 2009; Yin et al., 2005). However, there are pressing issues with data that need to be addressed, with limited data available for crop genotypes and performance across different environments and under different management techniques (White, 2009). Currently, restrictions with data result in many investigations into integrating modelling and genomics using the same dataset for both calibration and evaluation, which does not provide an independent assessment of the model (White and Hoogenboom, 1996). Additionally, although numerous major loci have been identified for crop physiological traits, there are still many genes that have yet to be detected. For example, in the case of wheat, with the genes regulating photoperiod sensitivity, vernalisation, earliness *per se* and stem height considered well enough understood to model their effects in gene-based models. Further genes, for instance governing grain size and protein concentration, are less well understood. However, for some genes, for instance those affecting photosynthesis, respiration and root-shoot partitioning, there is a lack of information. This could be a result of these processes being affected by large gene networks, by genes that have relatively minor effects or that inaccurate characterisation of genotypes has resulted in the non-discovery of these genes (White, 2006). The first

step in the process to progress gene-based modelling is to genetically characterise diverse wheat cultivars from different field trials (Hoogenboom et al., 2004).

The integration of genomics and crop models is still in its infancy. Considering the limitations of this approaches, this modelling may prove most effective when applied to analyse traits that are more important or processes that are environmentally stable or demonstrate easily quantifiable responses, for instance, the effect of temperature and photoperiod on phenology (White, 2006).

1.3.2.2 The Larger-than-Field Scale

Although initially crop models were developed and applied at the field scale over the short-term, recent research has prioritised the application of these models to assess climate change impacts, as well as potential mitigation and adaptation options, over the long-term at larger-than-field scales (Soussana et al., 2010; Ramirez-Villegas et al., 2012; Cammarano et al., 2017).

Crop models have also been used extensively in combination with climate scenarios generated by global climate models (GCMs) in an attempt to assess the effect of long-term projected climate changes on the cropping system. These include increased temperatures (Semenov & Shewry 2011; Stratonovitch & Semenov, 2015), changes in precipitation frequency and severity (Semenov & Halford, 2009; Richter & Semenov, 2005; Kholova et al., 2014), soil salinization (Asseng et al., 2001; van Ittersum et al., 2003) and increased CO_2 levels (Parry et al., 1999; Rosenzweig et al., 2014; Tao & Zhang, 2013; Tubiello et al., 2000).

For example, the crop model CropSyst was applied using climate change scenarios derived from GCMs to assess the effect of a doubling of CO_2 on the yields of six

crops under rotation at two sites in Italy (Tubiello et al., 2000). The simulations predicted that the changes in climate and increased CO_2 would result in reduced crop yields under current management practices, as a result of increased temperatures accelerating crop phenology and resulting in yield reductions of up to 40%. Application of the model to assess potential adaptation options indicated that planting spring-summer crops earlier and selecting winter cereal cultivars that took longer to reach maturity would prevent a reduction in crop yields at both sites. However, in order to maintain the current yields for irrigated crops, up to 90% more irrigation water was required under the projected increased temperatures. As the availability of water for irrigation in the future is likely to be restricted, this suggests that adaptation options may be limited for irrigated crops (Tubiello et al., 2000).

1.3.2.3 Limitations

Crop models have demonstrated to differ in their simulation of yield responses to climate change (e.g. Asseng et al., 2013). The reasons for these differences need to be established, so that crop models can be usefully applied (Challinor et al., 2005). Uncertainty - a lack of exact knowledge (Uusitalo et al., 2015) - in modelling can originate from a number of sources, including (i) model input variables (ii) model structure (i.e. model equations) and (iii) model parameters (Brun et al., 2006). For example, analysis of the mechanistic model, GLAM, demonstrated that the model's yield prediction was more sensitive to perturbations in climate inputs than crop parameters (Challinor et al., 2005), i.e. the input data was a larger source of uncertainty than the model structure or parameters. If the uncertainty associated with a particular model is quantified, then informed decisions can be made regarding the model outputs (Rosenzweig et al., 2013; Uusitalo et al., 2015). This relative

importance of crop model and climate vary spatially, however, so careful consideration needs to be given to the assessment of model uncertainty (Challinor et al., 2010; Porter et al., 2014). Non-climatic factors are not easy to characterise temporally and spatially at the larger-scale, so it is difficult to quantify relationships between these and crop yield. Additionally, the relative importance of climatic variables, e.g. temperature and precipitation, differs at broader scales. Across most crops and regions, temperature has been demonstrated to contribute more to uncertainty than precipitation (Lobell & Field, 2007; Lobell et al., 2008), with the temporal variability of precipitation reduced at broader spatial scales.

The uncertainty in crop model predictions can be quantified and assessed by model ensembles. To create an ensemble, a single model can be applied to produce multiple predictions by altering values of model parameters and/or inputs, with the variability between model outputs used as a measure of uncertainty (Tao et al., 2009; Tao & Zhang, 2013; Challinor et al., 2005; Iizumi et al., 2009). Multiple different crop models can also be applied to create a multi-model ensemble (e.g. Asseng et al., 2013; Martre et al., 2015). Using ensembles, the source of prediction uncertainty can be assessed. For instance, Asseng et al. (2013) demonstrated using a multi-model ensemble that a greater portion of the uncertainty in climate change projections could be attributed to crop models, than climate.

Model ensemble studies have demonstrated that the use of an average prediction produced by these multi-model ensembles, (Palosuo et al., 2011; Asseng et al., 2015), was better able to reproduce the observed crop temperature response of yield than any single model. The same conclusion was reached with respect to wheat

growth (Martre et al., 2015). The use of larger ensembles provides the opportunity to produce more rigorous and probabilistic results (Challinor et al., 2005; Tao et al., 2009; Tao & Zhang, 2013). For instance, one ensemble generated 18,000 simulation results to assess the impact of future climate change on Maize in the North China Plain, produced from a combination of one crop model applied to 10 climate scenarios, over 30 years, with 60 sets of crop parameters (Tao et al., 2009). This large number of ensemble simulations allows probability distributions to be generated from the results, allowing probabilistic predictions, for instance, the results predicted that there was a 60% probability that maize yields would decrease by 8.4% during the 2020s, relative to the baseline period. This probabilistic prediction could be a more useful quantification of simulation results for policy-makers and stakeholders (Tao et al., 2009).

Traditional crop simulation models typically require input data in large quantity and at high quality (Leenhardt et al., 2006), describing weather, soil properties and management decisions (Adam et al., 2010). Climatic inputs generated for the purpose of climate change assessment by GCMs are generated on the regional to global level. This is large-scale, coarse data, resulting in a mismatch of scales between the input data available for these applications and the point-scale, detailed crop models (Parry et al., 2004; Ramirez-Villegas et al., 2012; Adam et al., 2011). At the GCM scale, heterogeneity within the spatial grids is lost. However, spatial variability in weather within a region or country can be large, requiring smaller scales to capture (Chalinor et al., 2009; Van Bussel et al., 2011).

Policy decisions are made at the regional level, so this is frequently the scale of interest when simulating climate change impacts (Van Bussel et al., 2011). However, at this scale there is often a lack of data defining the spatial distribution of inputs required by crop models (Hansen & Jones, 2000). Model inputs, including climate, soil and management decisions, are often obtained from multiple different scales in such applications (e.g. Estes et al., 2013a), and where multiple models are used in impact assessment, data is scaled between field, farm and regional scale at which the individual models operate, adding further complexity and sources of uncertainty (Ewert et al., 2011). The impact of the scaling of input data on crop models is the subject of active research (Cammarano et al., 2017; Van Bussel et al., 2011; Hoffman et al., 2016; Ewert et al., 2011). Advances in remote sensing have permitted global observations to be made at high spatial and temporal resolution using satellites over large, regional areas (Baret et al., 2007), which offers promise for providing data for use with crop models at the larger scale (Baret et al., 2007; Guerif & Duke, 2000; Rodriguez et al., 2004; Estes et al., 2013b; Mo et al., 2005) and reducing the uncertainty associated with model outputs (Moulin et al., 1998; Houles et al., 2004).

In addition to inputs describing weather, soil properties and management decisions, the calibration of mechanistic models can require detailed phenological and growth observations over time (Challinor & Wheeler, 2008). This can make them difficult to calibrate and limited calibration can result in poor model performance (Angulo et al., 2013; Palosuo et al., 2011) . Limited calibration could produce a model that performs well for the data against which it was calibrated (e.g. yield under certain climatic conditions), but which arrives at that ‘right’ answer for the ‘wrong’ reasons. For

example, models that were able to simulate end-of-season crop components accurately, were able to do so without accurately simulating within-season growth (Martre et al., 2015). This can occur if model calibration is limited, allowing 'compensation errors' to occur when values are estimated for intermediate variables. In one example, accurate simulation of yield could be obtained through under-estimation of leaf area near anthesis and subsequent under-estimation of aboveground biomass, which was compensated for by over-estimation of the harvest index to an unrealistic value (Martre et al., 2015).

As discussed, the number of input variables, initial conditions and parameters required to setup, alongside the data required for sufficient calibration, by mechanistic models is often large, and this information can be lacking (either completely or at the scale of interest) (Jonscaap, 2006). New models can be developed for application on the scales at which climate inputs are produced (regional to global), with a focus on requirement of minimal calibration and input data required (e.g. GLAM, Challinor et al., 2004). In addition, existing, the re-assessment and simplification of existing complex, mechanistic models can be performed (Books et al., 2001; Crout et al., 2014). In attempting to explain crop growth and development, mechanistic models have become large and complex, containing numerous processes and parameters and can suffer from poor parameter identifiability - the ability for model parameters to be uniquely determined from measurable data (Brun et al., 2001). The key to resolving this issue is to identify and retain the aspects of the crop system that are essential, which will differ depending on the modeller's interest (Goudriaan and Van Laar, 2012). This process of model simplification – identification and removal of redundant parameters and descriptions

that do not contribute to model performance - has been suggested for existing mechanistic crop models and simplified versions of the existing mechanistic model, Sirius, have been developed for use at the regional (e.g. Brooks et al., 2001) and field scale (e.g. Crout et al., 2014).

Empirical crop models usually focus on the relationship between crop yield and climate, and have been demonstrated to perform better at broader scales, at which the climatic input data is provided (Lobell et al., 2010; Lobell & Field, 2007; Challinor et al., 2005). It has been argued that the relationship between climate and yield is more appropriately described by simpler means at coarse scales (Lobell & Field, 2007; Challinor et al., 2005).

Importantly, in addition to differences in simulations between mechanistic models themselves, application of empirical models alongside mechanistic models to assess the impact of projected climate change has also produced differing (Morin & Thuiller, 2009; Estes et al., 2013b), or even contrasting predictions (Giardin et al., 2008; Estes et al., 2013b). Generally, empirical models project larger climate losses (Giardin et al., 2008; Estes et al., 2013b). Empirical models have also been demonstrated to reproduce yield observations more accurately than a mechanistic model (Estes et al., 2013a; Estes et al., 2013b). This demonstrates the potential for empirical models to be utilised at the broader scales involved in climate change impact assessment (Estes et al., 2013a). A mechanistic model applied at the larger-scale had numerous potential sources of error, as a result of the large quantity and quality of input data required, initial values, requiring data to be obtained from multiple scales (Estes et al., 2013a). For these reasons, simpler empirical models

may be more appropriate for large spatial applications, due to their requirement for less detailed data.

Empirical models, however, have their own limitations. As they are developed to describe, rather than explain, the relationship between yield and climate, their performance may not be maintained under changing environmental conditions, outside the range in which the model was developed (Estes et al., 2013a; Lobell & Burke, 2010). They are also unable to account for important effects that mechanistic models are capable of accounting for, for example mitigation and adaptation, through management (e.g. sowing date) and phenology changes (Lobell & Field, 2007; Estes et al., 2013b; Morin & Thuiller, 2009). Mechanistic models predictions can therefore be more optimistic through their ability to simulate the beneficial impact of rising CO_2 concentrations on crop growth and phenotypic plasticity (Estes et al., 2013b). Empirical models may more accurately represent crop temperature sensitivities, which mechanistic models may under-estimate (Estes et al., 2013b; Rotter et al., 2011). Additionally, empirical and mechanistic models have been demonstrated to be sensitive to, and respond differently to, different data input error sources (Watson et al., 2015).

Currently, mechanistic models are the focus of ensemble and inter-comparison studies. However, empirical models should be considered as a complement to mechanistic models (Estes et al., 2013a; Estes et al., 2013b; Watson et al., 2015; Morin & Thuiller, 2009; Giardin & Tardif, 2008) for a complete picture of crop-climate responses captured by crop models, as these different model types have different data requirements and sensitivities (Watson et al., 2015; Estes et al., 2013b).

Therefore, both model types have a role to play to improve crop yield predictions (Watson et al., 2015). Application of multiple models in an ensemble offers the opportunity to combine the knowledge and processes contained within each (Challinor et al., 2013; Martre et al., 2015).

1.4 Aims & Objectives

As demonstrated by the literature discussed, crop models have the potential to be useful tools, in particular in addressing the challenges associated with climate change. However, discrepancies between model predictions have necessitated the quantification and assessment of uncertainty associated with model outputs, in order that the predictions they provide are useful (Rosenzweig et al., 2014). The formation of (multi-)model ensembles is key to achieving this, with probabilistic ensembles providing useful quantification of results for policy-makers and stakeholders.

Traditional mechanistic models were developed at the point-scale and are complex, requiring a large quantity of inputs, initial conditions and parameters to be provided (Adam et al., 2011). Because of their complexity, mechanistic models can provide guidance on trait identification and potentially provide physiological insight into key responses (e.g. Semenov et al., 2007). There is also the potential for gene- and QTL- based responses to be to simulating differences in cultivars, although this is especially limited by sufficient data, capturing sufficient variability in the target trait.

The point-scale nature of traditional mechanistic models creates a disparity in scales between the input data they require and that provided for climate change assessment (Parry et al., 2004). Calibration of model parameters can also be problematic at this larger scale. The development of new mechanistic models for

application on these scales with a reduced data and calibration requirement is possible, although assessment of existing mechanistic models for simplification to improve their applicability at larger-scales, by identification of redundant processes and parameters, can also be performed (Brooks et al., 2001; Crout et al., 2014).

At this broader-scale, empirical models have been demonstrated to be advantageous, through their reduced data requirements. In applications they have produced differing or even contrasting predictions to mechanistic models (Estes et al., 2013a; Girardin et al., 2008). Although much research has been focused on mechanistic models, including in application of multi-model ensembles, consideration of both model types will provide a more complete prediction (Watson et al., 2015).

As the categorisation of models is broad, this had led to differences in their classification amongst authors. For example, GLAM was classified a hybrid model by one author (Di Paola et al., 2016), but ‘mechanistic’ by others (e.g. Watson et al., 2015). As the number of adjustable parameters for a model are often unclear, it is necessary to consider other model metrics when assessing model complexity. Some mechanistic models are incredibly detailed, with many processes described and hundreds of parameters. However, it has been demonstrated that a more complex model - one with more parameters - does not produce better predictions.

The majority of research at the larger-than-field scale has focused on the long-term effects of climate change, and therefore has been aimed at the regional, country, area or global scale (Holzkämper et al., 2015). Little research has been aimed at the farm scale, with limited examples of models developed using farm observations, or investigation of the controlling factors for yield in the farm situation (Mirschel et al.,

2014). Farmers do not grow crops under research trial conditions. This results in a 'yield gap' between the potential yields for a crop under research trials, and the attainable yield of a crop under farming (Lobell et al., 2009). Development of models from farm-level datasets (rather than application of models developed at the field scale from field-level datasets), which has been neglected in current research, will be a focus of this thesis.

Considering the above, this thesis aims to answer the following research questions:

1. Can differences in wheat cultivar growth and development be similarly explained using simplified versions of an existing mechanistic model?
    - Is it necessary to have all currently available model parameters and modelled processes to describe these differences? Or are there processes simulated by the model that do not improve the ability of the model to predict growth and development of differing cultivars – i.e. that can be removed or simplified?
2. Which modelling approach (empirical or mechanistic) is suited to modelling yield at the farm scale using farm-level observations?
    - Is one approach better able to simulate farm-level yields? Or is there potential for both to provide insight?

To address these questions, this thesis aims to develop, analyse and contrast models of differing complexity applied at the farm and field scale. The specific objectives of the work are:

- To parameterise an existing, mechanistic wheat model for multiple cultivars using relatively detailed field level observations, identifying potentially redundant processes in this model using a reduction analysis (Chapter 3). The model that will be used is Sirius, which is introduced above (Section 1.3.1).
- Considering the results obtained in Chapter 3, to develop, parameterise and analyse for reduction, a mechanistic model of intermediate complexity using field level observations, for application at the field scale (Chapter 4).
- To develop, parameterise and validate both a simple empirical and a simple mechanistic model of wheat using farm level observations for application at the farm scale (Chapter 5).

It has been argued that models should undergo a systematic evaluation of their structure, which is one aspect that contributes to model uncertainty (Crout et al., 2014). Although previous simplification work has employed a more manual, time-intensive, expert consideration of processes within the model (Brooks et al. 2001), an automated method was employed here, considered more appropriate given the complexity of modern crop models.

Within a given model, the results of such an evaluation are dependent on the (quality of) data used to assess the relationships within the model and their contribution to model performance. This thesis therefore will expand on an initial model reduction analysis performed by Crout et al. (2014), for the Sirius model. In addition to considering the model structure, the work will be further expanded by considering

parameters describing cultivar differences (another source of model uncertainty). The datasets used will still consider within season measurements and multiple crop components, as in the work of Crout et al. (2014), but with a reduced number of observations and a larger number of cultivars, with a broad range of phenology. This will indicate whether the redundancies identified by Crout et al. (2014) are more widely applicable (i.e. the same processes are identified when additional data are considered), or are more specific to the data used in informing the reduction analysis (i.e. the processes identified differ, and therefore the identified reduced model has a restricted application), given the same systematic approach.

In summary, although the Sirius model has been the subject of earlier simplification attempts (Brooks et al., 2001; Crout et al., 2014), no other investigation has considered such a comprehensive search of both model processes and cultivar-specific parameters for reduction, in addition to the number of cultivars, under varying nitrogen applications.

This work is also novel in its consideration of farm-level statistics for model development, and consideration of the appropriate modelling approach. Rather than a ‘top-down approach’, i.e. simplifying models developed at the field scale using field level data, this thesis will focus on developing new models for use at the farm scale using observations made at the same level. This data source and scale appears neglected in current research (Mirschel et al., 2014)..

For clarity, the diagram below provides an overview of the models utilised within this thesis (Figure 1.3). To provide a more complete picture of their complexity, they are summarised by number of:

- modules (m) - a module is a section of the model used to describe a set of related (sub-)processes, e.g. vernalisation.
- variables (v) – total number of varying values used in model equations, e.g. thermal time.
- parameters (p) – total number of fixed values used to describe model setup e.g. soil characteristics such as soil depth, as well as number of fixed values used to differences in wheat cultivars, e.g. canopy extinction coefficient.

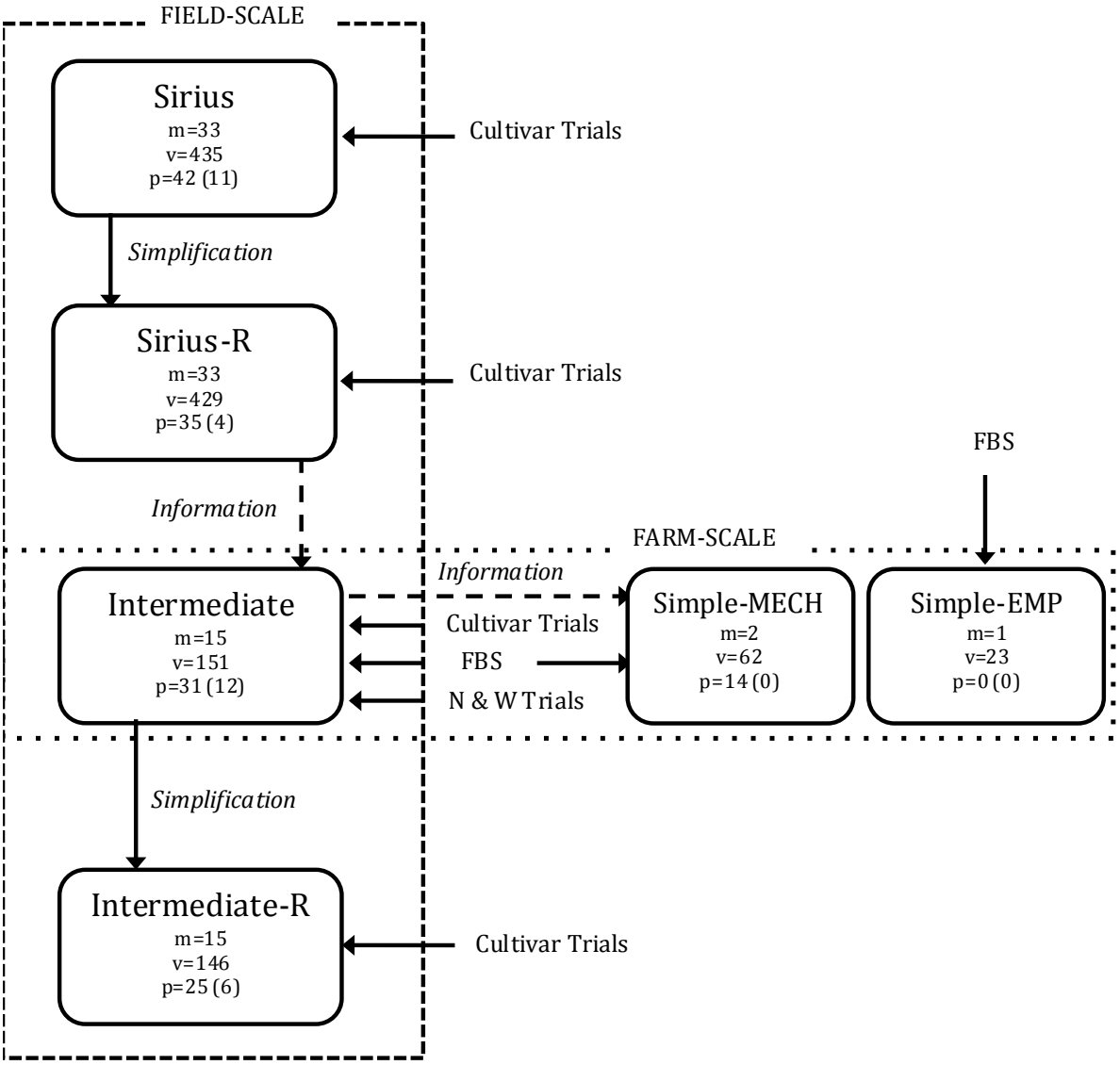


Figure 1.3 Models Utilised or Developed in this Thesis: including the scale (farm or field) at which they were applied (farm= - - -, field= . . .), datasets used (Cultivar Trials/N&W Trials/FBS), and whether they were developed through the process of model reduction (*Simplification*) or informed from the application of other models (*Information*). M=number of modules that form model. V=number of variables model consists of. P= total number of parameters (number of parameters used to describe cultivars). FBS; Farm Business Survey. N & W Trials; Nitrogen and Water-Limitation Trials.

As established, the classification of model type is broad, in this thesis the following classifications will be used:

- **empirical**: to describe a model comprised entirely of statistical relationship(s)

- **mechanistic**: to describe models used and developed that attempt to describe processes, no matter the level of detail considered

The mechanistic models will be distinguished by their level of complexity, as judged by their metrics (Figure 1.3). As per the above definitions, the model previously identified by authors as both a ‘hybrid’ and ‘mechanistic’ model, GLAM, would here be classified as a mechanistic model, of intermediate complexity. The models in this thesis include five mechanistic models (Sirius, Sirius-R, Intermediate, Intermediate-R and Simple-MECH) and one statistical model (Simple-EMP). All consider nitrogen- and water- limited growth. They range from complex (Sirius, Sirius-R), to intermediate (Intermediate, Intermediate-R), to simple (Simple-MECH, Simple-EMP) in complexity based on the number of modules, variables, total number of parameters, as well as number of parameters considered cultivar-specific. The empiricism of the mechanistic models increases with each model reduction (Sirius-R, Intermediate-R) and new design (Intermediate, Simple-MECH).

2 Methods

2.1 Overview

This chapter outlines the modelling and analysis techniques used in this thesis. The software, notation and conventions are described, as well as statistical analyses employed. Model calibration and validation are introduced. A summary of the methodology applied in each chapter is provided (Section 2.10), alongside references to the use of individual statistics throughout.

The author did not collect the data described and used within this chapter and therefore the associated fieldwork methods are not described. A brief summary of methods is given where appropriate, with relevant publications cited.

2.2 Software

The following software was used for the development and analysis of models:

- **OpenModel Version 2.3.0** (©2015 University of Nottingham; www.openmodel.info) – a windows-based program developed for the specification, solution, parameterisation and visual and numerical analysis of mathematical models.
- **Minitab® 16** (©2010 Minitab Inc.; www.minitab.com) – a statistical analysis program which can be used to generate basic statistics, perform regression, analysis of variance and cluster analyses on data input into a worksheet.

Data were provided in spreadsheets using Microsoft Excel (©2010 Microsoft Corporation). These spreadsheets were edited and imported into the OpenModel and Minitab software packages.

2.3 Model Notation

Model calculations require quantities from field, laboratory or other modelling research for use either as inputs to mathematical equations or for comparison with model outputs. Model notation and convention is summarised in Figure 2.1.

A model requires **inputs** (e.g. rainfall), quantities that may vary over time, which are obtained from observations in the field, laboratory or previous modelling research. In addition, non-variable quantities known as **constants** (e.g. specific leaf nitrogen) and **parameters** (e.g. extinction coefficient of the crop canopy) need to be defined. Although both constants and parameters do not alter within the simulation (over time), parameters can vary between simulations (with differing model setup). Therefore, parameters can be 'optimised' to achieve the best fitting model. Within the model, **intermediate variables** are calculated from input variables, constants and parameters during model execution. They may be an intermediary step in calculation of the model output, or represent a real quantity. The **model output** is the quantity calculated by the model, which is directly comparable to the observed output. It is a function of the input variables and defined constants and parameters. Model performance is assessed by comparison of the modelled and observed output. Parameter optimisation is performed by minimising the difference between the two outputs.

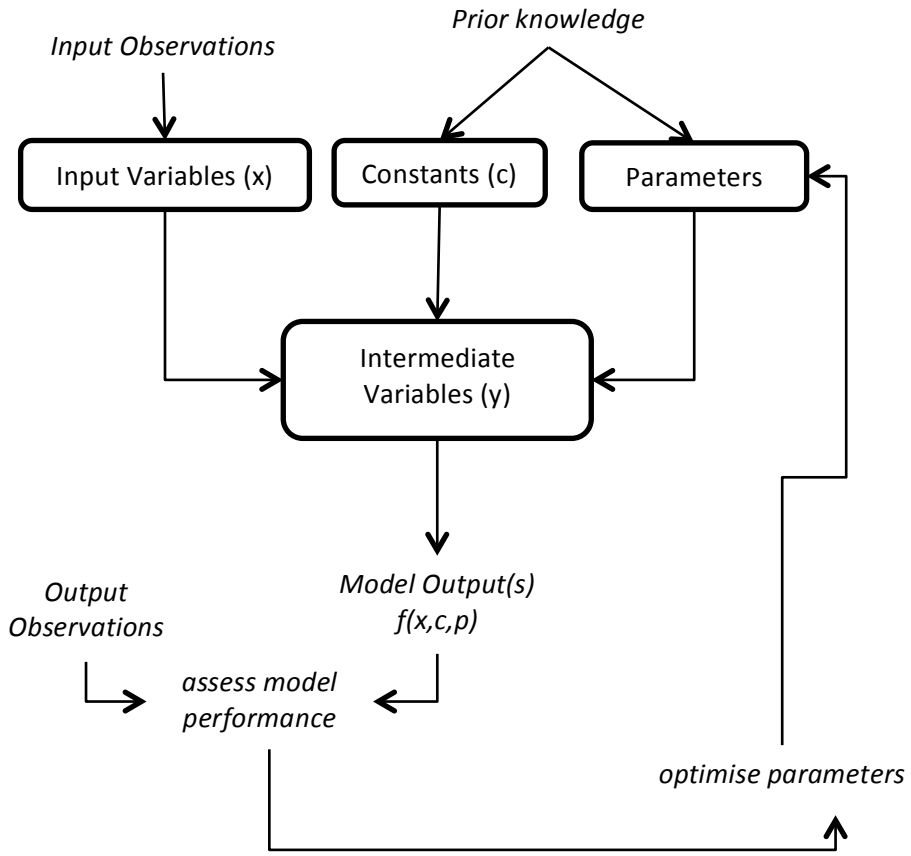


Figure 2.1 Schematic overview of notation and convention used in mathematical modelling.

2.4 Model Construction

2.4.1 Statistical Model

The statistical software Minitab® was used to select variables by stepwise regression for inclusion in the model when their variance ratios were significant at the 5% level. The model developed using this method is described in Section 5.4.

2.4.2 Mechanistic Models

Mechanistic models were constructed in OpenModel (OM), in which models can be specified as equations using a conventional mathematical syntax, linking inputs,

parameters and constants to calculate model variables, and subsequent outputs. The software allows the construction of models in modular form, with related sets of equations specified in separate modules. This allows a complex model to be constructed from a number of interconnected modules. External data can be imported into datasheets for use as model inputs or for comparison between modelled and observed outputs. OM also accepts external data in spatial form, as regular 2-dimensional grids. The mechanistic models applied or developed in this thesis are described in Sections 1.3.1 (Sirius and Sirius-R), 4.2 (Intermediate and Intermediate-R) and 5.5 (Farm-MECH).

2.4.2.1 Model Evaluation

The mechanistic models in this thesis are dynamic – i.e. simulate the crop system over time. Dynamic, mechanistic models require solving of a differential equation, such as Equation 2.1.

$$\frac{dY}{dt} = k\frac{dB}{dt} \qquad \textbf{Equation 2.1}$$

The complexity of modern dynamic models requires this to be solved numerically, replacing the infinitesimal time dt with a finite time-step Δt. In this thesis, the numerical integration method used is Euler, which takes a user-defined time-step and calculates the model output based on the values at the previous time-step. Euler is not recommended for the solution of differential equations, due to the propagation of errors if there are large changes in the system during the time-step. However, it is simple, easy to implement and widely used by crop models, in which the daily time step prevents the modelled system experiencing large changes (Stockle et al., 2003).

2.5 Basic Model Analysis

The performance of a model with respect to the observed data is measured by the agreement between the data and model predictions - a model's 'goodness of fit'. All model analysis assumes that data are normally distributed. A number of different measures of model fit are used throughout this thesis.

The total sum of squares (SS_{tot}) is defined as the sum over all data points of the difference between the data point and the mean (Equation 2.2). This is the intrinsic variation of the dataset about its mean. This difference can be weighted for each individual data point to produce a weighted total sum of squares (WSS_{tot}), by dividing by the error on the data point (Equation 2.3). Data points with smaller errors are given more importance in the calculation. The amount of variation from the mean that can be explained by a model can then be assessed using the explained sum of squares (WSS_{exp}) (Equation 2.4).

$$SS_{tot} = \sum_{i=1}^{n}(O_i - \bar{O})^2 \qquad \textbf{Equation 2.2}$$

$$WSS_{tot} = \sum_{i=1}^{n}\left(\frac{O_i-\bar{O}}{W_i}\right)^2 \qquad \textbf{Equation 2.3}$$

$$WSS_{exp} = \sum_{i=1}^{n}\left(\frac{P_i - \bar{O}}{W_i}\right)^2 \qquad \textbf{Equation 2.4}$$

Where n is the number of observations, O_i is the *i*th observation, $\bar{O}$ is the mean of the observed values, W_i is the weight associated with the *i*th observation and P_i is the *i*th predicted value. The higher the value of WSS_{exp}, the better the fit of the model. However, the function most used when assessing model fit is the weighted residual sum of squares, WSS_{res}, which represents the variation not explained by the model (Equation 2.5).

$$WSS_{res} = \sum_{i=1}^{n} \left(\frac{O_i - P_i}{W_i}\right)^2 \qquad \textbf{Equation 2.5}$$

The lower the value of WSS_{res}, the better fit of the model, and therefore it is often the quantity minimised in parameter optimisation. However, without the relative values of WSS_{tot} and WSS_{exp}, WSS_{res} is meaningless. Therefore, the r^2 statistic is often used to infer the best fitting model (Equation 2.6).

$$r^2 = \frac{WSS_{exp}}{WSS_{tot}} \qquad \textbf{Equation 2.6}$$

r^2 represents the fraction of the variation that is explained by the model, with a value of 1 representing a perfect fit, with the model perfectly predicting the observations.

Statistics such as r^2 are sensitive to the range of (an) independent variable(s) and are not appropriate for use with datasets in which these variables encompass a narrow range. In these situations, these statistics can indicate low model predictive ability, even in the presence of good agreement between observed and modelled values. An alternative is the use of mean absolute error (MAE)(Equation 2.7) or mean percentage error (MAPE)(Equation 2.8) to assess error in model predictions. These statistics can be weighted. By definition, MAE is unit specific, and so cannot

be compared between data series of differing units. However, as a relative measure, expressed as a percentage, MAPE can be used to compare the error between data series of differing units.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|O_i - P_i| \qquad \textbf{Equation 2.7}$$

$$MAPE = \frac{100}{n}\sum_{i=1}^{n}\left|\frac{O_i - P_i}{O_i}\right| \qquad \textbf{Equation 2.8}$$

$$wMAE = \frac{1}{\sum W_i}\sum_{i=1}^{n} W_i|O_i - P_i| \qquad \textbf{Equation 2.9}$$

$$wMAPE = 100\,\frac{\sum_{i=1}^{n} W_i(|O_i - P_i|)}{\sum_{i=1}^{n} W_i O_i} \qquad \textbf{Equation 2.10}$$

Where n is the number of observations, O_i is the *i*th observation, $\bar{O}$ is the mean of the observed values, W_i is the weight associated with the *i*th observation and P_i is the *i*th predicted value. Model performance is assessed using MAE and MAPE in Section 5.6, with the weighted versions of these statistics utilised in Chapters 3 and 4.

2.6 Model Selection

The statistic specifically used in model selection was the adjusted r^2 statistic (r^2_{adj}), a version of the r^2 statistic that considers the number of adjustable parameters (s) in

the model (Equation 2.11). This statistic allows comparison of the explanatory power of models with different numbers of parameters, producing a measure of the relative quality of models for a given dataset. The preferred model is the one with the greatest r^2_{adj} value. This statistic is used in Section 5.6 to assess the relative performance of the empirical and mechanistic models.

$$r^2{}_{adj} = 1 - \frac{(\sum(O_i - P_i)^2)/(n-1)}{(\sum(O_i - \bar{O})^2)/(n-s-1)}$$

Equation 2.11

$$r^2{}_{adj} = 1 - \frac{(\sum(O_i - P_i)^2)/(n-1)}{(\sum(O_i - \bar{O})^2)/(n-p-1)}$$

Equation 2.12

2.7 Model Parameterisation

A sophisticated iterative parameter estimation method was used to optimise model parameters; Metropolis-Hastings (MH) (Haario et al., 2001).

MH uses a Markov Chain Monte Carlo (MCMC) algorithm to estimate parameters using prior information about a parameter, alongside the data. When used with the appropriate prior distribution and likelihood function, MH can be used to infer a Bayesian estimation. Such methods facilitate the estimation of large numbers of parameters for large computer models and locate the global minimum more reliably. MH generates a random walk based on a proposal distribution and a criteria for rejecting some of the proposed moves or ending the search, described below. These criteria can be defined by the user to optimise parameterisation performance.

Extensive preliminary assessment of parameterisation performance was used to determine the appropriate setup of the search procedure for each implementation. Specific setup details are included in the relevant chapter. A brief explanation of the search procedure and the influence of the criteria is included here.

The MH algorithm randomly ‘walks’ the parameter space, as defined by the user-specified distribution and constraints, from the user-specified initiating parameter value. The ability for the user to specify prior parameter distributions allows literature and expert knowledge to inform the search. These prior distributions can take the form of a normal or uniform distribution, with lower and upper bounds (Figure 2.2). A uniform distribution is uninformative, assigning equal probabilities to each value in the range, but use of a normal distribution, with differing means and standard deviations, allows informed parameter searches. The further a value is from the mean, the lesser its probability of being selected. Values within one standard deviation of the mean have a 68% probability of being selected, those within two standard deviations have a 95% probability. If little information is known about the parameter that is being estimated, then a uniform distribution or a normal distribution with a larger standard deviation can be used, to represent ignorance about that parameter. Upper and lower bounds can be used to constrain the estimates to a reasonable range, e.g. only positive values for parameters describing time elapsed.

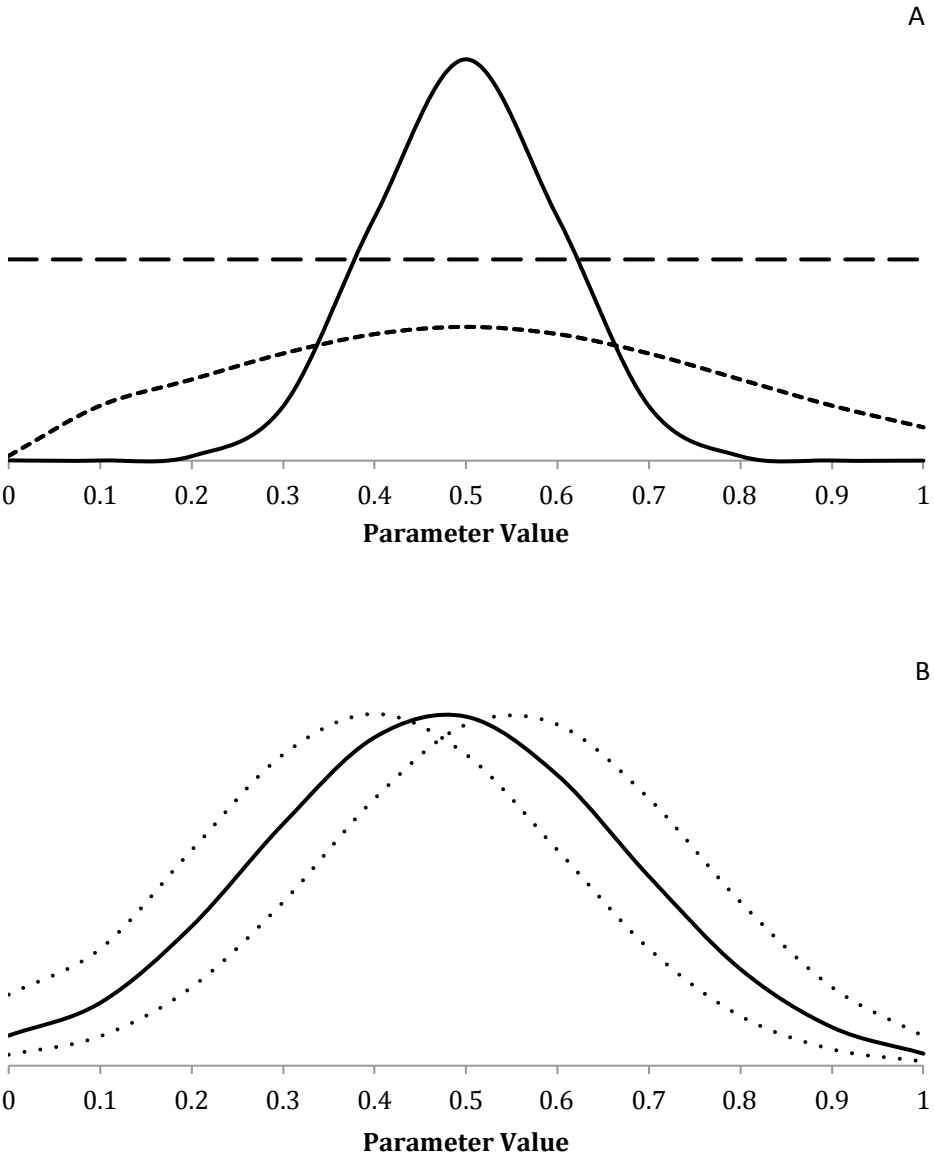


Figure 2.2 Examples of parameter prior distributions. All distributions are constrained between 0 and 1. A uniform distribution is uninformative, but use of a normal distribution, centered around different mean values, and with different standard deviations, allows informed parameter searches. (A) Uninformative (- - -), narrower (-------) and wider(- - -) informative distributions using altered standard deviations around an identical mean. (B) Informative distributions using different means, but identical standard deviations.

The proposal distribution controls the 'walk' through parameter space, setting how they are likely to move per step. It can be fixed, or allowed to adapt during the search to improve search efficiency, as described by Haario et al (2001). At each

step during the walk, parameter values are accepted if they exceed a user-specified improvement in model fit, assessed by probability calculated as a function of SS_{res}. The decision-making process of the algorithm is summarised in Figure 2.3. An important feature of MH is ability to accept 'bad' moves, i.e. those that worsen the model fit. This prevents the algorithm getting stuck in local minima (Figure 2.4).

Briefly, the algorithm;

- picks a starting point in the search space (= set of parameter values)
- calculates the probability of those parameters
- then, until the stopping criteria are met:
    1. picks a new, candidate point at random (but near to the previous point)
    2. calculate the probability of this candidate point
    3. calculate the acceptance ratio (candidate/previous)
    4. if the value of this ratio is greater than 1 (i.e. the candidate point is more likely than the previous point), accept the candidate point and return to 1
    5. if the value of this ratio is less than 1, accept the candidate with the probability equal to this ratio and return to 1

Figure 2.3 Summary of the MH methodology

Initially, the parameter value selected is highly variable, resulting in relatively larger changes in the SS_{res} (Figure 2.4). After a certain number of iterations, in this example approximately 1,200, the algorithm converges on a parameter value. If insufficient iterations are performed, there is a risk that only a local, rather than the global, minimum in SS_{res} will be identified (Figure 2.4). This SS_{res} minima would be the best

SS_{res} - parameter combination, which produces the convergence. However, 'underneath' this SS_{res} minima, the parameters and SS_{res} are still walking the parameter space. The parameter search can be setup to continue for a set number of iterations, or until after a set number of non-improvement steps. Whilst the latter approach reduces the risk of obtaining a parameter value that is a local minima, it can significantly extend the parameterisation run time.

The variability or uncertainty of the parameter estimates produced by the MH search were assessed using the coefficient of variation (CV), which is defined as the ratio of the standard deviation (σ) to the mean (μ) (Equation 2.13).

$$CV = \frac{\sigma}{\mu}$$ **Equation 2.13**

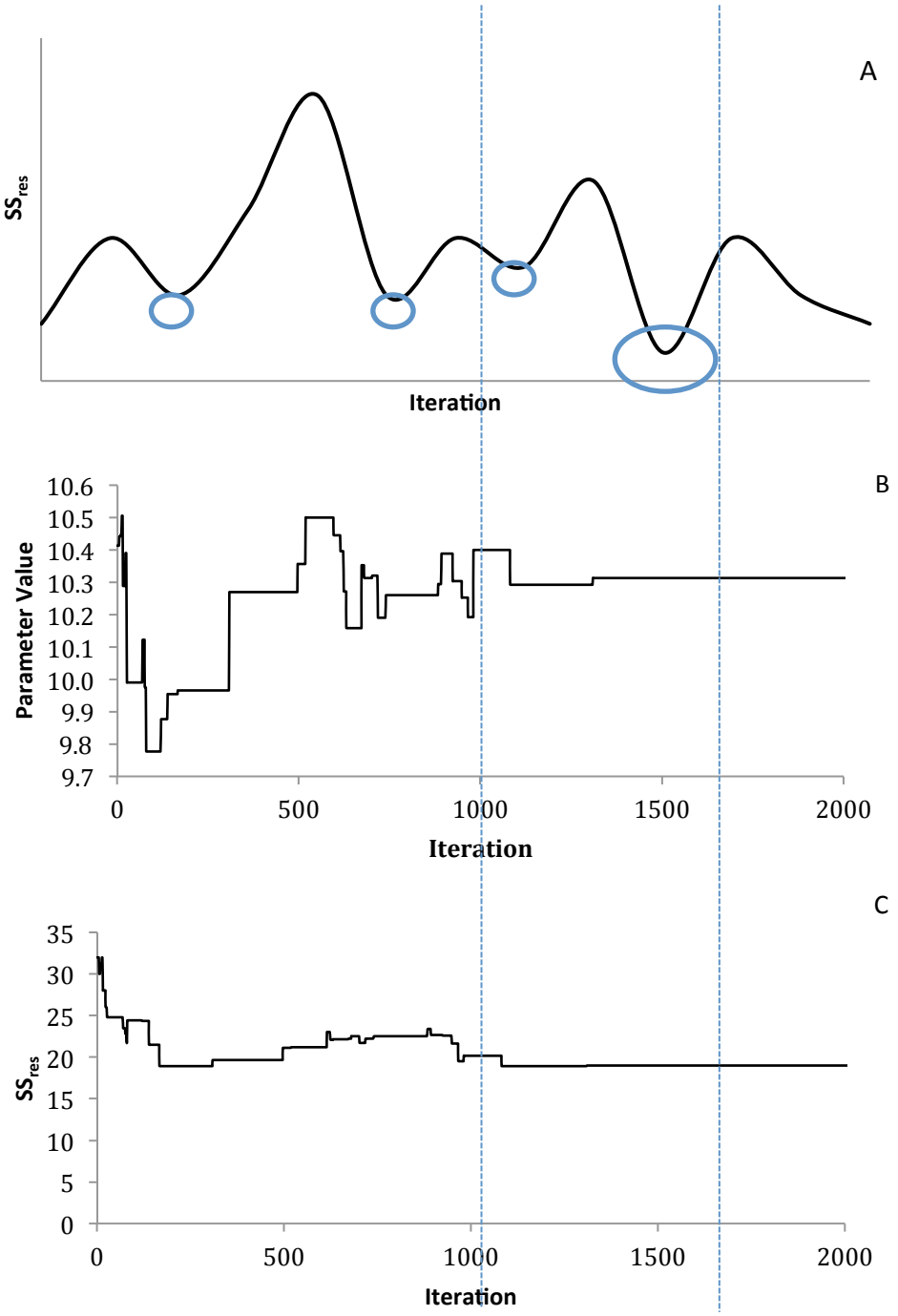


Figure 2.4 A graphical illustration of the progress of model parameter estimation. (A) Sufficient iterations must be performed to ensure that global (larger circle) and not local (smaller circle) minima in SSres are identified. (B) Change in parameter value with iteration, and (C) the associated alteration in SSres. If only 1,000 iterations were performed, the global minima identified at 1,500 iterations would be missed.

In addition, the sensitivity (S) of a model to a certain parameter (P) can be assessed by:

$$S = \frac{\Delta F / F(P = P_0)}{\Delta P / P_0}$$ **Equation 2.14**

Where F is the (Sum of Squared Residuals) SS_{res} of the parameterised model, ΔF is the change in SS_{res} relative to the change in parameter, ΔP, from a baseline value, P_0.

The SS_{res}, and CV are used to assess model parameterisations in Chapters 3 and 4. In addition, Sensitivity (in association with a correlation matrix generated during parameterisation) was used to aid in identifying key parameters for the more complex model in Chapter 3.

2.8 Model Reduction

Model reduction was explored using an automated method, a full description of which is available (Cox et al., 2006; Crout et al., 2009). Briefly, the methods analyse the effect of selected model variables on model performance, by replacing these variables with constants and comparing the reduced model against the selected observational data. If a variable was important for model prediction, it would be expected that replacing it with a constant value (for all trials), would be detrimental, worsening the agreement between observations and predictions. The method of model reduction described below was used to determine simplified versions of both the Sirius (Section 3.3.3; Sirius-R) and Intermediate (Section 4.4; Intermediate-R)

models, considering both model variables and parameters describing cultivar differences.

Initially, variables to be excluded from the reduction analysis were identified - these variables were implemented in the code for diagnostic or output purposes, were not involved in modelled processes and therefore did not affect model function. Due to the computational expense of reduction methods, a screening analysis was used to further refine the list of remaining candidate variables, by replacing each variable individually with a fitted constant. Subsequently a multi-factorial method was employed, which replaced variables in combination with the fitted constants obtained in the screening analysis. A truly exhaustive search, in which every possible combination of the candidate variables is considered, was not possible given the number of variables. Instead, a MH search was employed, which incorporates a random element, as described below.

At each step of the MH walk, model predictions were compared to the observed values to calculate a pseudo-likelihood. A step was accepted if:

$$\frac{Q_{trial}}{Q_{current}} > r$$ **Equation 2.15**

Where the $Q_{current}$ and Q_{trial} are the pseudo-likelihoods of the currently accepted and trial reduced model combinations, respectively. r is a random value between 0 and 1. Moves which reduce model likelihood, can be accepted to enable escape from local minima in the search space. The probability of accepting a bad move is the ratio of

the trial and current pseudo-likelihoods, and for each iteration this is compared to the randomly generated r.

The pseudo-likelihoods were normalised to unity over the models considered and a replacement probability was calculated for each variable by summing the normalised pseudo-likelihoods for the models where the given variable was replaced over the model evaluations. These replacement probabilities were reported at designated intervals to ensure they had stabilised within the number of iterations performed.

Belief in the model was related to the weighted WSS_{res}, by calculation of a pseudo-likelihood (Q_i) (Equation 2.16). This was determined for each reduced model.

$$Q_i = exp\left(\frac{-\ln(0.5)(WSS_{res_{full}} - WSS_{res_i})}{\alpha}\right) \qquad \textbf{Equation 2.16}$$

Where $WSS_{res_{full}}$ and WSS_{res_i} are the weighted residual sums of squares for the full model and the i^{th} reduced model, respectively. α is a constant controlling how changes in WSS_{res} affect belief in the model. α is the change in WSS_{res} which alters the belief in the model by a factor of two and was set at 5.0% of the value of $WSS_{res_{full}}$. Previously it has been demonstrated that altering this informal constant value (2.5%, 5%, 10%) does not have a significant effect on the result and its interpretation, therefore the central value was selected for use in this analysis (Crout et al., 2014).

2.9 Datasets

A number of datasets were utilised in model calibration and validation. They included field trial datasets, with observations from six locations and 18 different wheat cultivars, with water-limited, nitrogen-limited and potential treatments. Additionally, datasets generated from surveys at the farm level were also utilised.

2.9.1 Farm Datasets

At the farm level, the England and Wales Farm Business Survey (FBS) collects financial and physical data for all types of farms across England and Wales to underpin both national policy requirements and contribute to the European Farm Accountancy Data Network (DEFRA, 2013a). This dataset was used to develop both a mechanistic (Section 5.5; Farm-MECH) and an empirical model (Section 5.4; Farm-STAT). In total, 3,367 yield observations from 700 farms over the period 2005-2010 were available. Additional data for each farm obtained from the database included; farm and wheat cropped area, wheat yield, output value of the wheat crop, variable (seed, fertiliser, crop production and other costs) and fixed (labour, machinery, land and contract) costs, as well as farm / farmer characteristic data (farmer age, farmer education level, organic status of farm and organic enterprises on farm, plus an estimated livestock waste, i.e. manure/slurry, applied to the wheat crop).

The farm location is only identified within the data to the nearest 25x25km within the UK's national grid reference system. Monthly mean values of maximum and minimum temperatures (°C), sunshine hours (hours), and rainfall (mm) were obtained on a 5x5km national grid basis from the UK Met Office for October 2005 to

July 2010 (MetOffice, 2014), and values for the 25x25km grid (farm locations) were estimated as an average of these 5x5km data. Although daily maximum and minimum temperatures were available (°C), daily sunshine hours (hours) / radiation (MJm^{-2}), and daily rainfall (mm) were not freely available for the farm locations.

2.9.2 Field Datasets

A number of field trial datasets were used. These included single cultivar United Kingdom nitrogen (Gillett et al., 1999) and New Zealand drought response (Jamieson and Semenov, 2000; Jamieson et al., 1998a) trials (Table 2.1), as well as a comprehensive multi-cultivar Nitrogen Use Efficiency (NUE) trial with both UK and French sites (Table 3.2) (Gaju et al., 2011). The single cultivar nitrogen and drought response trials included detailed observations of crop growth (Table 2.1), whilst the NUE trials had far fewer observations, but for a much larger number of cultivars (Table 2.2). As a result of their numerous observations, and inclusion of both water- and nitrogen- limiting conditions, the single-cultivar trials were used in the testing of newly developed models' ability to simulate biomass, LAI and grain yield over time under both potential and limiting conditions (Section 4.3.1.1). The NUE trial datasets provided far fewer observations over the crop growth period, but a far greater number of cultivars were observed, providing the opportunity to assess a model's ability to parameterise for, and model, different cultivars (Sections 3.3.1 and 4.3.1.2). Previous experimental work has demonstrated that the 16 cultivars that were included in this dataset have a broad range of photoperiod response and vernalisation requirement, and their range of anthesis dates is similar to that observed in wheat breeding programs (He et al., 2012).

Daily maximum and minimum temperatures (°C), radiation (MJm^{-2}), and rainfall (mm), wind (ms^{-1}) and vapour pressure (kPa) were obtained for all sites.

Table 2.1 Summary of datasets from nitrogen and drought trials used in model development, parameter estimation and testing.

Dataset	Organisation	County	Latitude and Longitude (°)	Years	Treatments	Cultivars	Observations (Number of)
Sutton Bonington	University of Nottingham	UK	52.83 N 1.25 W	1993 1994	Restricted growth: - 0 kg ha^{-1} - 90 kg ha^{-1} - 190 kg ha^{-1}	1 (winter): Mercia	**Time series of:** Biomass (97), Grain (27), LAI (53) **Additional data:** Final Leaf Number (3), Anthesis Date (3)
Lincoln	New Zealand Institute for Crop and Food Research Ltd	New Zealand	43.36 S 172.28 E	1992 1993	Drought response: - 616 mm (180 kg ha^{-1}) - 163 mm (180 kg ha^{-1}) - 96 mm (180 kg ha^{-1}) - 14 mm (180 kg ha^{-1})	1 (spring): Batten	**Time series of:** Biomass (48), Grain (35), LAI (59)

Table 2.2 Summary of datasets from NUE trial used in model development, parameter estimation and testing.

Dataset	Organisation	County	Latitude and Longitude (°)	Years	Treatments	Cultivars	Observations
Sutton Bonington	University of Nottingham	UK	52.50 N 1.14 W	2007 2008	Potential growth: - 210 kg ha^{-1} and 210 kg ha^{-1} Restricted growth: - 0 kg ha^{-1} and 30 kg ha^{-1}	15 (winter) 1 (spring)	**Time series of:** Biomass (14), LAI (8) **Additional data:** Grain (4), Anthesis Date (4), Final Leaf Number (4), Phyllochron (4)
Clermont-Ferrand	INRA	France	45.46 N 3.09 E	2007 2008	Potential growth: - 240 kg ha^{-1} and 240 kg ha^{-1} Restricted growth: - 40 kg ha^{-1} and 40 kg ha^{-1}	15 (winter wheat), 1 (spring wheat)	**Time series of:** Biomass (8) **Additional data:** Grain (4), Anthesis Date (4)
Estrées-Mons	INRA	France	49.08 N 3.00 E	2007 2008	Potential growth: - 240 kg ha^{-1} and 210 kg ha^{-1} Restricted growth: - 50 kg ha^{-1} and 50 kg ha^{-1}	15 (winter wheat), 1 (spring wheat)	**Time series of:** Biomass (8) **Additional data:** Grain (4), Anthesis Date (4)

3 An Existing Mechanistic Model

3.1 Introduction

Application of modern, mechanistic models at the larger-than-field scale, in the assessment of climate change impacts has highlighted a key limitation of these complex models – their requirement for a large quantity and quality of input data (Estes et al., 2013a).

The combination of increased knowledge of underlying processes and enhanced computer power have facilitated the development of these large and complex crop simulation models. However, increasing model size and complexity does not necessarily produce a 'better' model, and large and complex models with numerous parameters can suffer from poor parameter identifiability - the ability for model parameters to be uniquely determined from measurable data (Brun et al., 2001).

Model parameters are estimated through minimisation of a criterion, producing the best agreement between the observed and simulated data. Whilst manual ad-hoc tuning of individual parameters was previously possible, in modern crop modelling, the complexity of models necessitates the use of sophisticated, automated algorithms in model parameterisation and analysis (e.g. He et al., 2012). Over-parameterised models are those for which multiple parameter solutions can be obtained through repeated optimisation from different starting points – i.e. the parameter values estimated are subject to the initiating value provided (Guérif et al., 2006).

This is increasingly becoming an issue, not only in the application of these models at larger-than-field scales, where less (detailed) data is available for both model input and calibration, but in determining meaningful cultivar-specific values for predicting differences between crop cultivars.

Ideally a parameterisation would produce parameter values that were both identifiable and realistic for the cultivar being described, ensuring that the model is capable of simulating the behaviour of a cultivar under conditions outside that which it was calibrated under. A good parameter value, as assessed by the parameterisation process, may produce a poor prediction if it does not accurately represent the characteristic it is describing (Brun et al., 2006). There is no universal approach to model parameterisation, and often model developers do not provide any guidance or specific details on the parameter estimation setup used during published research.

The use of Bayesian estimation methods, in which estimation of parameter values can be informed using altered prior distributions, is one approach to aid in producing both identifiable and realistic values. However, this technique is time consuming and subjective (Brun et al., 2001). Obtaining identifiable parameters values can also be complicated by a lack of sensitivity of the observations to the parameters (Saltelli et al., 2000; Varella et al., 2010). Therefore, assessing the influence of parameter variation on modelled outputs – through a sensitivity analysis – can aid in identifying parameters with the greatest influence, and thus identify the main targets for parameter estimation. This approach is regularly used (Varella et al., 2010).

Rather than simply focusing on estimating the parameters that have the greatest impact on model outputs, an alternative approach is to improve parameter identifiability through model reduction (Crout et al., 2009; Crout et al., 2014). This approach assesses the influence of modelled processes on the model's predictive ability, with those that do not contribute to the prediction considered redundant. This analysis can lead to a reduced model, which represents fewer modelled processes, and requires fewer inputs and parameters to be determined for its implementation, improving it's applicability at larger-than-field scales (Brooks et al., 2001).

One such mechanistic crop model, Sirius, has been the subject of such simplification. Sirius is a typical mechanistic crop model, simulating wheat growth and development on a daily time-step. Detailed descriptions of the model have been published (Jamieson and Semenov, 2000; Jamieson et al., 1998a; Lawless et al., 2005), and an introduction to the model is given in Section 1.3.1.

Brooks et al. (2001) performed a sensitivity and structural analysis of the Sirius model, replacing key model components describing the canopy, soil water balance and evapotranspiration with simplified, empirical descriptions. This 'meta-model' had a reduced number of parameters, but was able to produce similar yield predictions to the original model at sites within the UK. In addition, the simplified process enabled weather variables to be input on a monthly, rather than daily time-step, through the use of cumulative weather variables. These simplifications make the meta-model more easily applicable on a regional scale, where such detailed weather data are not available (Brooks et al., 2001). In addition, the resulting model had a faster run time,

making it more appropriate for regional modelling exercises, requiring multiple simulations.

A second study applied a systematic model reduction technique to Sirius. A powerful alternative to the manual 'tuning' of parameters which is the approach more commonly utilised and allowing a more complete exploration of parameter values and combinations. (e.g. Semenov et al., 2007; Brooks et al., 2001). This approach identified 16 model variables (14% of the total number) as potentially redundant (Crout et al., 2014). The simplified model, in which these variables were replaced by constants, performed better than the original model. Similarly to Brooks et al. (2000), redundancies were noted in processes describing evapotranspiration and vernalisation. Although the simplified model of Brooks et al. (2001) considered unlimited nitrogen, descriptions of nitrogen uptake and remobilisation were also identified as redundant in the analysis of Crout et al. (2014), who considered both nitrogen- and water- limited trials.

3.1.1 Aims

Considering the above, the aims of this chapter are to;

- analyse the identifiability of cultivar parameters in Sirius using a dataset of 16 wheat cultivars (2.9.2)
- produce and assess parameterisations for the 16 wheat cultivars for;
    - physiological accuracy
    - identifiability of parameters, by considering; (i) the influence of initiating value, (ii) the influence of informed prior distributions, and (iii) the correlation between parameters being estimated. The model will be

considered over-parameterised if; (i) parameter values are subject to their initiating value, (ii) cannot be influenced by use of informed prior distributions, and (iii) there are a large number of significant correlations between the parameters being estimated.

- further investigate the potential of the Sirius model for reduction, extending the previous work by applying the comprehensive reduction technique devised by Crout et al. (2014), but considering both model processes and cultivar-specific parameters, and using observations for an increased number of cultivars, under varying nitrogen applications, to ensure the simplified model is able to capture cultivar differences
- identify descriptions and processes that could be excluded to form a model of intermediate complexity, using the results of a reduction analysis

Table 3.1 A Description of the Sirius2005 cultivar parameters, their constrained ranges during parameterisation and their influence on crop growth and development.

Parameter	Units	Constraints		Description	Influence
		Lower	Upper		
Thermal Time					
TTSOWEM	°C Days	100	250	Thermal time from sowing to emergence	Crop emerges and growth begins when accumulated thermal time exceeds this value.
TTANBGF	°C Days	50	190	Thermal time from anthesis to the beginning of grain fill	Grain filling begins when accumulated thermal time from anthesis exceeds this value.
TTBGEG	°C Days	400	650	Thermal time from the beginning of grain fill to the end of grain fill	Grain filling ends when accumulated thermal time from beginning of grain filling exceeds this value.
PHYLL	°C Days	70	150	Phyllochron	Controls leaf emergence and duration of leaf growth, lag and senescence phases. Also used to define anthesis.
Canopy					
Amax	m^2	0.0014	0.01	Potential maximum leaf size	The last five leaves have variable potential leaf sizes, increasing to this value.
LF_{min}	Leaves	4	11	Minimum possible leaf number	Calculation of final leaf number.
LF_{max}	Leaves	13	28	Maximum possible leaf number	Calculation of final leaf number.
K_e	-	0.36	0.78	Canopy light extinction coefficient	Calculation of potential biomass growth.
Daylength					
SLDL	Leaves $HourDaylight^{-1}$	0	3	Daylength response	Calculation of final leaf number.
Vernalisation					
VAI	$°C^{-1}$	0	0.01	Response of vernalisation rate to temperature	Calculation of vernalisation progression.
VBEE	Day^{-1}	0	2	Vernalisation rate (1/days) at 0 deg. C	Calculation of vernalisation progression.

3.2 Method

Sirius 2005 was transported to OpenModel using source code obtained from the model developers (P.Martre & M.Semenov, *pers. comm.*). This allowed a thorough model parameterisation and analysis to be performed. Cultivar parameters were identified from these files. All other model parameters were fixed at their default values, as specified.

The dataset used in the parameterisation contained biomass and yield observations over time for 16 cultivars in 2007 and 2008 at one site in the UK (Sutton Bonington) and two sites in France (Clermont Ferrand and Estrees-Mons) (Gaju et al., 2011). Two nitrogen treatments were applied with the aim of achieving potential and restricted growth. At Sutton Bonington (SB), additional observations were made of leaf area index (LAI), final leaf number (FLN) and phyllochron. Anthesis date was also recorded at all sites. Previous experimental work has demonstrated that the 16 cultivars have a broad range of photoperiod response and vernalisation requirement, and their range of anthesis dates is similar to that observed in wheat breeding programs (Table 3.2)(He et al., 2012).

Table 3.2 Characterisation of Photoperiod Response, Vernalisation Requirement and Average Yield and Average Flowering Date of the 16 Cultivars under NUE trials at Sites in the UK and France (He et al., 2012; Gaju et al., 2011).

Cultivar	Photoperiod Response[a]	Vernalisation Requirement[b]		Yield (t ha^{-1})	Anthesis Date
		0-8 weeks	4-8 weeks		
Alchemy	>1524	-	278	7.2	04 Jun
Arche	>1572	557	156	6.9	28 May
Beaver	>1476	-	-	6.6	04 Jun
CF9107	940	-	0	6.1	25 May
CF99102	1116	-	124	6.3	27 May
Consort	>1508	-	-	6.7	03 Jun
Paragon	>1669	290	120	6.4	01 Jun
Perfector	>1556	-	-	6.9	31 May
Quebon	>1604	-	694	6.5	31 May
Recital	312	-	253	5.6	19 May
Renan	1134	-	545	5.6	26 May
Rialto	882	-	236	6.7	01 Jun
Robigus	>1588	-	173	7.1	01 Jun
Savannah	>1540	-	322	7.1	02 Jun
Soissons	411	-	376	6.3	21 May
Toisondor	627	-	202	6.7	26 May

[a] Degree-days difference in heading dates in long days (20h photoperiod) and short days (10h photoperiod).

[b] Difference in degree-days in heading dates between non-/partially and fully vernalized plants, as determined on plants transplanted in the filed under long days after either 0, 4, or 8 weeks of vernalization under controlled conditions. Hyphens indicated that plants did not head.

In addition, some analysis was performed using a dataset that contained more detailed time-series observations of biomass, LAI and yield for one winter wheat cultivar (Mercia) in the UK (Sutton Bonington) and one spring wheat cultivar (Batten) in New Zealand (Lincoln) (Gillett et al., 1999). Daily maximum and minimum temperatures (°C), radiation (MJm^{-2}), and rainfall (mm), wind (ms^{-1}) and vapour pressure (kPa) were obtained for all sites for model inputs. Soil parameters were based on site observations (Gaju et al., 2011; Gillett et al., 1999). Parameter estimation was performed as described in Sections 2.7 and 2.8. A weighted merit

function was used, with the values of 10% (biomass, grain) and 20% (LAI), subject to a minimum value was applied of 500gm^{-2} for biomass and grain yield and 1 m^{2}m^{-2} for LAI. These values were selected as the estimated standard error of these observations, based on previous experience with crop analysis datasets (Crout et al., 2014). Assessment of weighted squared residuals was performed to ensure that no data points had an excessively high contribution to Weighted Residual Sum of Squares (WSS_{res}).

Specifically, in the initial round of parameter estimation, the setup included uninformative parameter prior distributions were specified with the estimation stopped if there was no improvement after 1000 steps, using a WSS_{res} reduction threshold of 0.01 to denote improvement. An adapting proposal was specified to achieve the desired acceptance rate of 25%. The parameter estimation was setup to allow the simultaneous parameterisation of all cultivars, moving the parameters in 16 groups (one for each cultivar). Constraints were applied to the parameter estimates as detailed in Table 3.1. These boundary values are assigned to encompass values documented in both published literature and previously parameterised cultivars (He et al., 2012), where available, and which would encompass the full range of values that could be expected for the cultivars in this dataset (*O. Gaju, pers. comm)*.

Sufficient observations per cultivar were not available to allow the splitting of the dataset into calibration and validation subsets. Therefore an independent assessment of the model parameterisations was not possible. Instead, final leaf number and phyllochron observations (where available) were used to assess the parameterisations, although these only provide an assessment of the phenology sub-model. Weighted mean absolute error (wMAE), mean absolute percentage error

(wMAPE) and the coefficient of variation (CV) were used to assess parameterisations. Additionally, the parameterisation was assessed for physiological credibility, by comparing with either previously calibrated values and known physiological and phenological information.

In order to assess the identifiability of cultivar parameters, four independent rounds of parameterisation were conducted, initiated at differing starting points in the parameter space (i.e. with differing initial values of the parameters). These starting points were based on previously published calibrations to include values describing cultivars with a range of characteristics (He et al., 2012). Parameter correlations produced during these parameterisations were used to identify parameter interactions and a sensitivity analysis was performed to identify key cultivar parameters. For each individual parameter, the constrained range was explored using 10 'steps' from the minimum to maximum possible parameter value. At each parameter value, the model was re-run to generate the associated sensitivity.

A model reduction analysis was performed as described in Section 2.8.

3.3 Results and Discussion

3.3.1 Cultivar Parameterisation

The four independent rounds of estimation (R1-4) achieved average mean weighted absolute percentage error (wMAPE) values of 31, 29, 27 and 25% for the 16 cultivars, respectively (Figure 3.1). For some parameters, for example the extinction coefficient (K_e), there was little variation in the average estimated value between rounds of estimation (0.47-0.50) (Table 3.3). However, parameters such as the daylength response (SLDL) were less identifiable, with more variable average estimated values for the 16 cultivars (Figure 3.3).

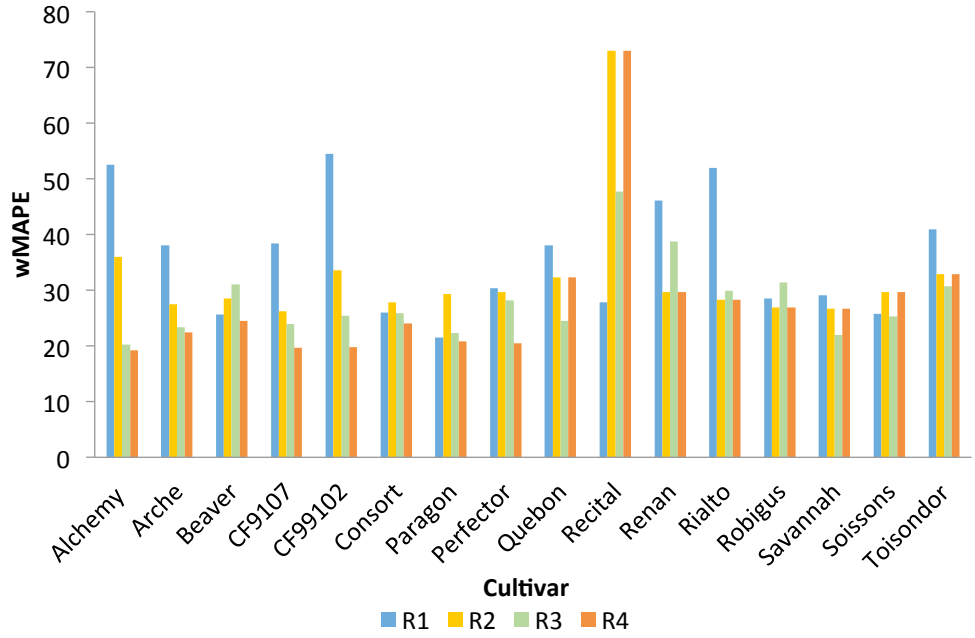


Figure 3.1 Weighted Mean Absolute Percentage Error (wMAPE) values for each cultivar achieved by the four independent rounds of estimation (R1-R4). Average wMAPEs of 31%, 29%, 27% and 25% were attained by R1, R2, R3 and R4 respectively. Cultivars graphed in alphabetical order.

Within the rounds of estimation, however, SLDL estimates showed relatively less variation between cultivars (CV<=7.4%)(Table 3.3). Parameters with the most variable estimates between cultivars within the rounds of estimation included those describing maximum potential leaf number (LF_{max}), potential maximum leaf size (A_{max}), and vernalisation response (VAI and VBEE) (Table 3.3). VAI estimates showed the greatest variability, with CV values of 10-46.7%.

Table 3.3 Average estimated parameter values for 16 cultivars over four independent rounds of estimation (R1-R4). The estimated (Est.) and coefficient of variation (CV) values represent the average for all 16 cultivars in that round.

	R1		R2		R3		R4	
	Est.	CV (%)	Est.	CV (%)	Est.	CV (%)	Est.	CV (%)
LF_{min}	8.8	4.0	9.0	3.1	9.4	3.9	5.4	11.2
LF_{max}	17.9	8.7	22.9	3.7	17.7	11.4	21.5	7.1
A_{max}	0.005	20.5	0.006	2.2	0.003	18.2	0.003	19.7
K_e	0.47	5.9	0.48	3.4	0.48	6.1	0.50	5.8
PHYLL	135	2.5	113	2.5	127	3.8	103	2.5
SLDL	0.16	6.4	0.57	3.4	0.22	7.4	1.38	5.8
TTANBGF	145	5.9	100	4.2	131	8.1	82	9.9
TTBGEG	532	6.0	496	3.8	490	7.2	533	6.6
TTSOWEM	177	6.5	150	3.5	160	6.0	166	6.9
VAI	0.002	39.4	0.004	10.0	0.001	21.7	0.005	46.7
VBEE	0.01	10.9	0.04	3.2	0.005	17.7	0.04	14.4

Across the four rounds of estimation, the lower overall wMAPE was generally attained through a better agreement between modelled and observed LAI, to which the majority of error in predictions were attributed. The most accurate predictions were made for anthesis, with an average wMAPE of 2.4% (Figure 3.5).

The use of altered prior distributions to inform the parameter estimation was explored for less identifiable parameters, to assess the impact this had on the fitted value that the parameterisation produced. By default, parameter prior distributions are described using normal distributions, with factors of 1 and 1,000 (of the initiating value) to describe the mean and standard deviation of the distribution, respectively. This results in an uninformative prior distribution, and therefore an uninformed

estimation of that parameter. The implementation and effect of such factors is demonstrated in Figure 3.2. Even at lower factor standard deviations (0.5, 1 and 2), the effect on the prior distribution can be clearly seen. The effect of a standard deviation of 87.5 °C Days (factor of 1) for example, is to loosely constrain the parameter estimates to the range 87.5°C Days – 262.5 °C Days, with approximately 68% of values being selected from this range.

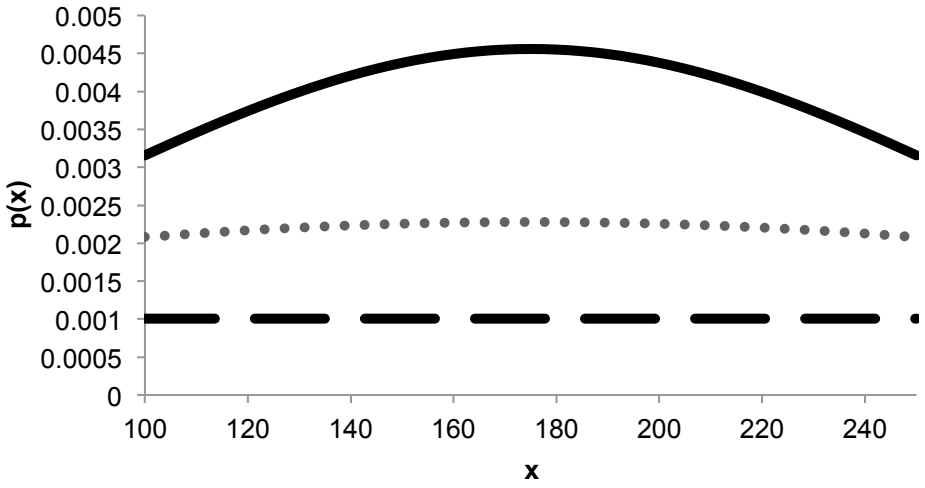


Figure 3.2 An example prior distribution for the parameter TTSOWEM, whose values were constrained in the range 100°C Days to 250 °C Days. Distributions shown here are for an initiating parameter value of 175 °C Days, with a mean of 175 °C Days (a factor of 1) and standard deviations at factors of 0.5 (87.5 °C Days), 1 (175 °C Days) and 2 (350 °C Days) of the initiating value.

Ultimately the use of informed distributions it did not prove very effective (Figure 3.4), with estimated parameter values remaining dependent on starting value. Therefore, default distributions were assigned for all the parameterisations presented here, and multiple independent rounds of estimation were performed.

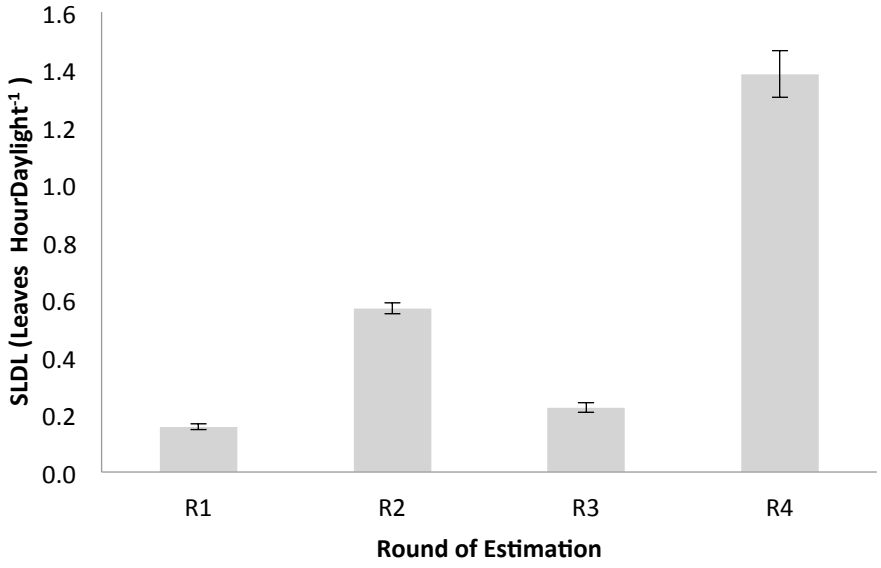


Figure 3.3 Average estimated values of the daylength response parameter (SLDL, Leaves HourDaylight^{-1}) for 16 cultivars over four rounds of independent estimation (R1-4). Error bars represent standard deviation of parameter estimate.

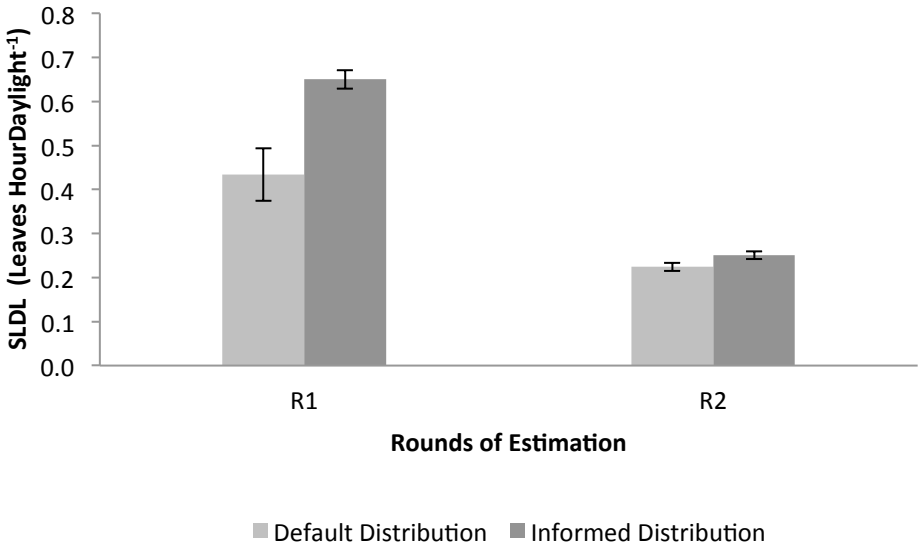


Figure 3.4: Example of values for the daylength response parameter (SLDL, Leaves HourDaylight^{-1}) estimated under differing parameter estimation setups. Initiating and estimated parameter values produced over two independent rounds of estimation (R1 and R2), with no prior alterations (default) and informed prior alterations (informed). Values were initiated at 0.5 and 0.2 for R1 and R2.

For each cultivar, the parameterisation that achieved the lowest wMAPE was selected from the four independent rounds for further analysis.

Total biomass (g m^{-2}), grain yield (g m^{-2}) and LAI were estimated with an average wMAPE of 27, 22 and 36%, respectively. The overall wMAPE of the 16 cultivars ranged from 19.2% (Alchemy) to 30.7% (Toisondor). Comparison of observed and predicted values for PHYLL and FLN, demonstrated that the parameterised model generally under-predicted FLN (wMAE = 2 leaves, wMAPE = 13%), and over-estimated PHYLL for the 16 cultivars (wMAE = 11.6 days, wMAPE = 10%). For the selected parameterisation for each cultivar, the parameter values are graphed in Figure 3.6 & Figure 3.7.

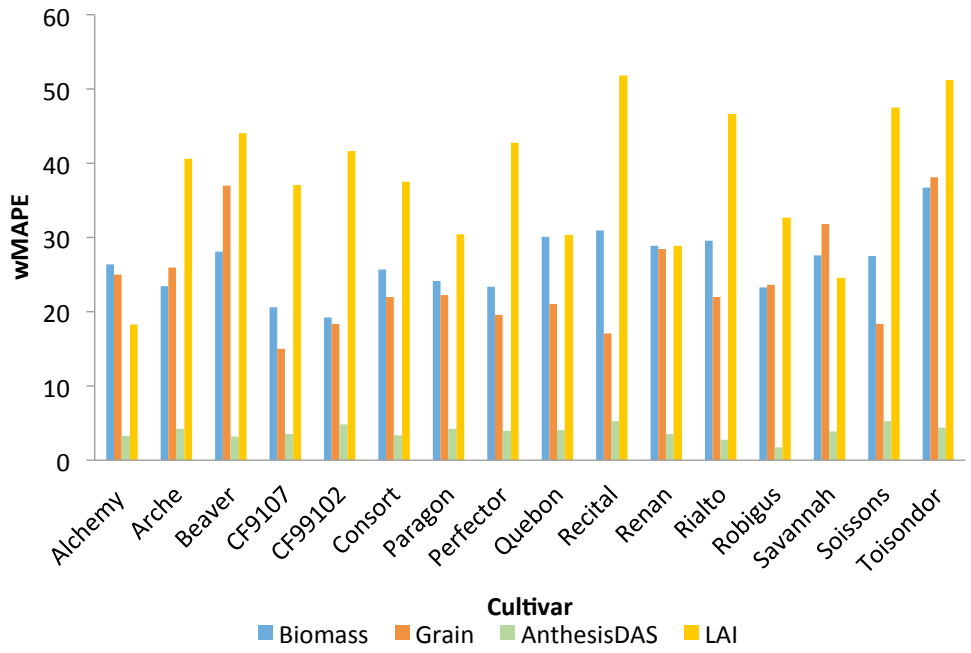


Figure 3.5 Weighted Mean Absolute Percentage Error (wMAPE) of biomass, grain yield, anthesisDAS and LAI of the best fitting parameterisation for each cultivar. Cultivars graphed in alphabetical order.

The cultivar-specific parameters of the phenology sub-model have previously been calibrated for these cultivars (He et al., 2012) and observations exist for a number of

the cultivar-specific parameters (Table 3.4). Estimates of absolute minimum leaf number (LF_{min}) encompassed a similar range (4 – 7.3 leaves) as these previously calibrated values. LF_{max} estimates however, were considerably higher (Figure 3.6), with the lowest estimate (13.8 leaves for Quebon), similar to the highest estimate achieved in previous calibrations. Difficulties were identified with LF_{max} estimation by He et al. (2012), as a result of this parameter having a low sensitivity index and relatively high level of interactions with other parameters. LF_{max} was one parameter identified here as having a relatively large coefficient of variation during parameterisation (Table 3.3).

The range of estimates for the phyllochron, PHYLL, (87 – 122 °Cd) were similar to observed variation in phyllochron for wheat (75 – 120 °Cd), although the values estimated previously were narrower (100 – 127 °Cd) (Figure 3.6). SLDL ranged from 1.12 to 1.85 leaves per hour of daylight, slightly higher than the range previously estimated, which varied from 1.08 to 1.57 leaves and substantially higher than published values (Table 3.4). The cultivar classified as least sensitive to daylength (Recital, SLDL=1.08 leaves) was assigned the second highest daylength response parameter value in this estimation (Figure 3.6). Renan, which had a relatively strong daylength response, was fitted with the greatest SLDL value (Table 3.2).

The response of vernalisation to temperature – VAI – ranged from 0.001 – 0.01 d^{-1} and was the most variable parameter (Table 3.2). This was also noted in the previous calibration, with the authors concluding that different values of VAI could achieve identical or similar model outputs. The second vernalisation parameter, describing vernalisation rate – VBEE – ranged from 0.019 – 0.067 d^{-1} $°C^{-1}$, which was higher than the range of observed values. Cultivars with no vernalisation

requirement – Paragon and Arche – were estimated to have relatively low VAI values. Consort, which demonstrated a strong vernalisation response during experimental trials (Table 3.2) was estimated to have the greatest VAI and second largest VBEE value, although similarly responsive Perfector was estimated to have a relatively low VBEE value (Figure 3.6).

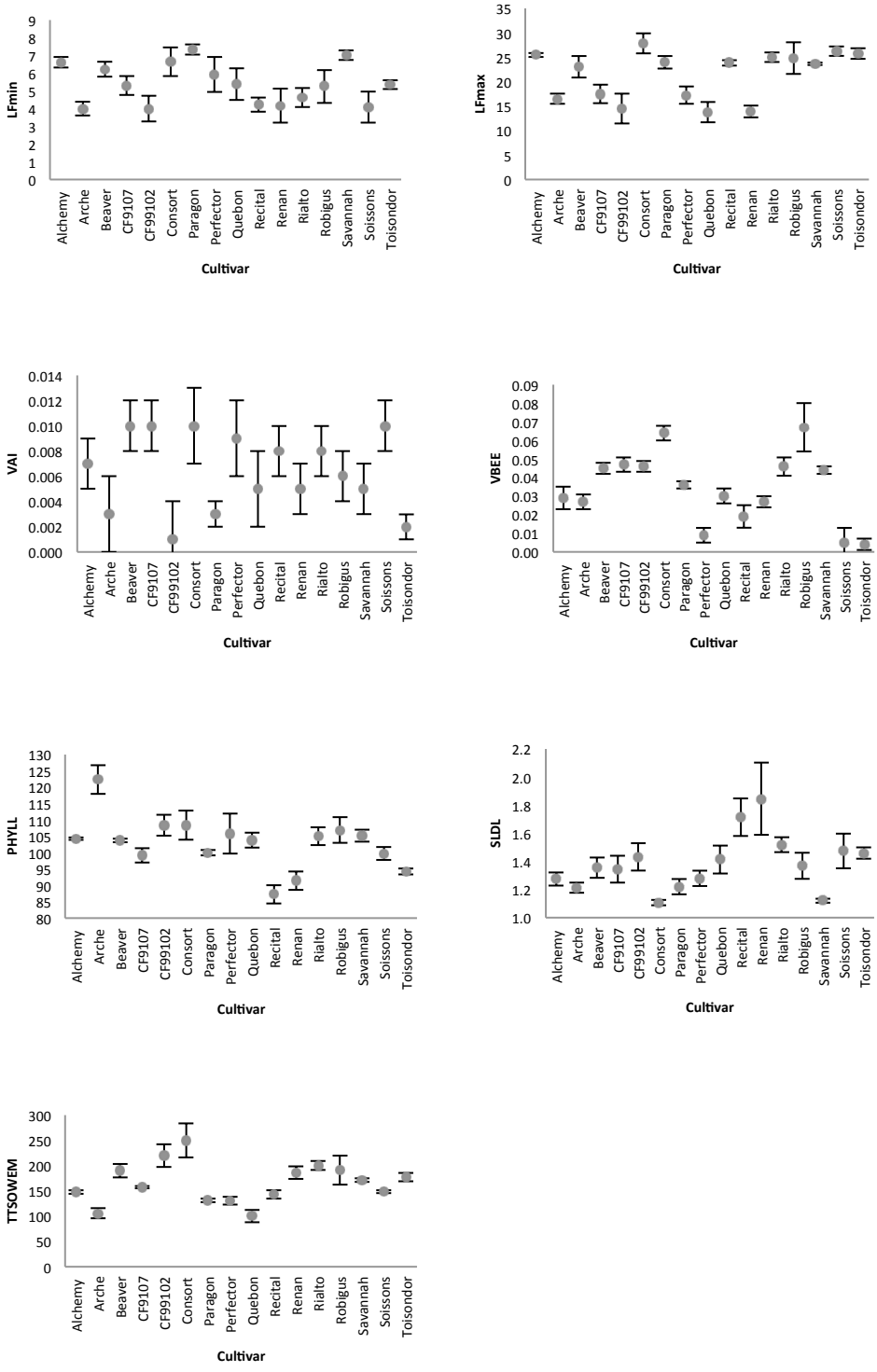


Figure 3.6 Estimated values of the cultivar-specific parameters of the phenology sub-model for the 16 cultivars. Error bars represent standard deviation of parameter estimates. Cultivars graphed in alphabetical order.

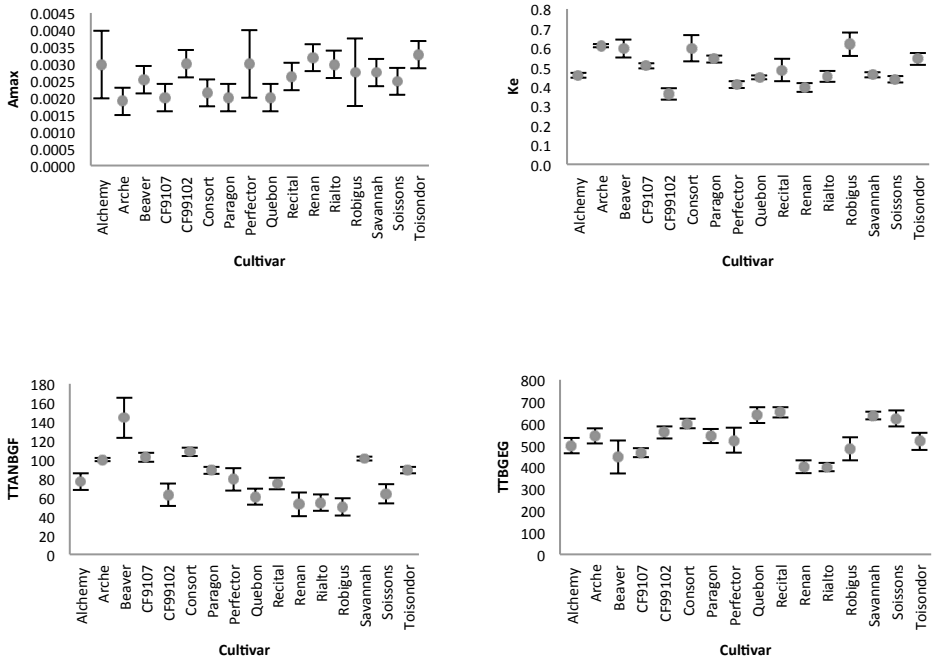


Figure 3.7 Estimated values of the cultivar-specific parameters of the dry matter and canopy sub-models for the 16 cultivars. Error bars represent standard deviation of parameter estimates. Cultivars graphed in alphabetical order.

Cultivar-specific parameters from outside the phenology sub-model were all within the ranges of observed values. K_e ranged from 0.40 – 0.62, which was within the observed variation in wheat varieties. A_{max} estimates (0.0020 - 0.0033m^2) were within the lower end of the observed range (Table 3.3). The thermal time constants, TTSOWEM, TTANBGF and TTBGEG described the thermal time between sowing and emergence, anthesis and the beginning of grainfill and grainfill duration, respectively. Their estimates were fitted across the constrained ranges, with observations for the thermal time from anthesis until the end of the grain filling period (410-875°Cd), similar to the estimated summed values for TTANBGF and TTBGEG (450 – 794 °Cd) (Table 3.3).

Table 3.4 Previously observed ranges of values for cultivar-specific parameters. Obtained from SiriusQuality forge (http://www1.clermont.inra.fr/siriusquality/).

Parameter	Unit	Range	References
PHYLL	°Cd	71-133	(Asseng et al., 2002; Frank and Bauer, 1995; Giunta et al., 2001; Ishag et al., 1998; Mossad et al., 1995)
A_{max}	m^2	0.0022-0.0088	(Fischer et al., 1998; Motzo and Giunta, 2002; Shearman et al., 2005)
K_e	-	0.36-0.78	(Calderini et al., 1997; Green, 1989; Miralles and Slafer, 1997; Muurinen and Peltonen-Sainio, 2006; Shearman et al., 2005; Yunusa et al., 1993)
RUE	g DM MJ^{-1}	1.2-2.8	(Acreche et al., 2009; Calderini et al., 1997; Miralles and Slafer, 1997; Muurinen and Peltonen-Sainio, 2006; Shearman et al., 2005; Yunusa et al., 1993)
SLDL			(Allison and Daynard, 1976; Holmes, 1973; Levy and Peterson, 1972; Rahman and Wilson, 1977; Slafer and Rawson, 1994)
VAI	d^{-1} $°C^{-1}$	0.0003-0.004	(Brooking and Jamieson, 2002; Brooking, 1996; Robertson et al., 1996)
VBEE	1/d	0.007-0.02	(Brooking and Jamieson, 2002; Brooking, 1996; Robertson et al., 1996)

3.3.2 Parameter Analysis

The parameterisations generated for the 16 cultivars were used to perform a sensitivity analysis by individually exploring parameter values, as detailed in 3.2. The example shown here for the cultivar Alchemy was typical of the responses of the 16 cultivars (Figure 3.8 & Figure 3.9).

The model was least sensitive to changes in the values of LF_{max} and VAI, with most cultivars showing no (S=0, as in the example of Alchemy) or minimal, sensitivity to these parameters (S<0.1) when the values of these parameters were individually explored using the cultivar parameterisations. Overall, the greatest sensitivity was demonstrated to changes in the parameters PHYLL, SLDL and LF_{min}, across the

range of values explored (Figure 3.8). Sensitivity to the vernalisation rate parameter (VBEE), whilst large in magnitude (S>1), was only noted when a value of 0 Day^{-1} was explored. Of the remaining parameters, the analysis indicated that the model was least sensitive to parameters describing the time from anthesis to the beginning of the grain filling period (TTANBGF) and grain filling duration (TTBGEG) (S<0.1, Figure 3.9).

The sensitivity analysis performed here assumes parameter independence and therefore does not account for interactions between the parameters. A correlation matrix generated from the best fitting parameterisation for the 16 cultivars indicated a large number of highly significant ($p<0.001$) parameter inter-correlations (Table 3.5), which means the results of the sensitivity analysis (and parameterisations) must be cautiously interpreted.

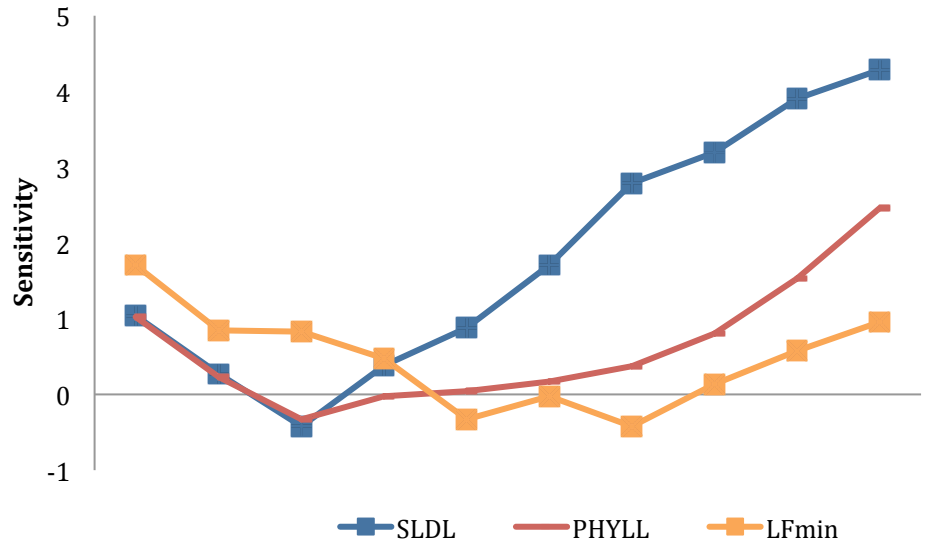


Figure 3.8 Sensitivity (S) of model outputs (biomass, yield, LAI and anthesis date) during exploration of the parameter space for Alchemy (winter wheat). Parameters to which the model demonstrated greatest sensitivity to are graphed (maximum S>1).

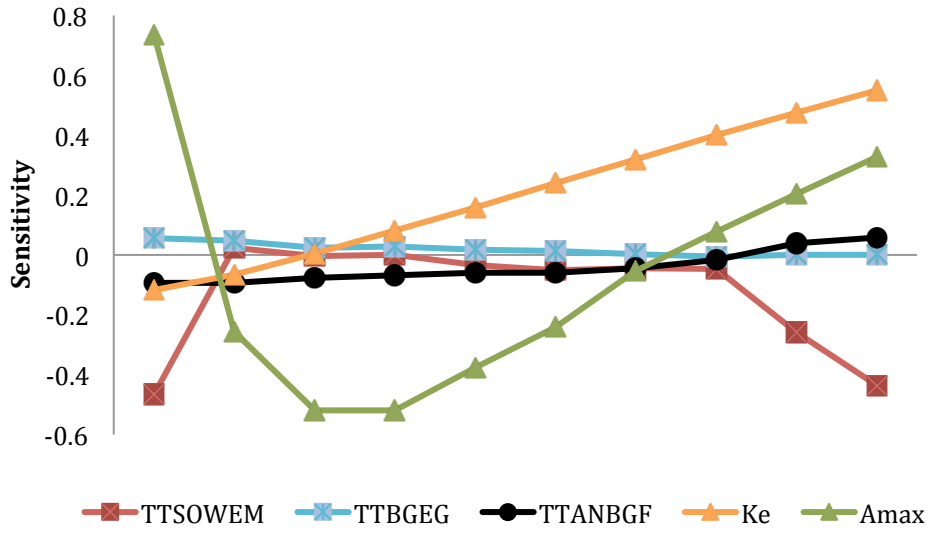


Figure 3.9 Sensitivity (S) of model outputs (biomass, yield, LAI and anthesis date) during exploration of the parameter space for Alchemy (winter wheat). Parameters to which the model demonstrated less sensitivity to are graphed (maximum S<=1).

For example, model outputs were found to be relatively insensitive (S< 0.1) to a number of parameters included in the calculation of vernalisation – VAI and LF_{max}. Additionally, the model only demonstrated sensitivity to another vernalisation parameter – VBEE – when it was set to zero. In this instance, the lack of effect does not necessarily indicate that the process of vernalisation, and its associated parameters, are not important in the model. The progression of vernalisation (VPROG) is a linear function of vernalising soil temperatures and the cultivars response to those temperatures (VAI and VBEE). Although vernalisation is complete when VPROG=1, it can also be considered complete if the primordia number (PRIMORDNO) exceeds the potential number of leaves (POTLFNO). PRIMORDNO is calculated simply as twice the number of leaves plus four, whilst POTLFNO is a function of LF_{max}, LF_{min} and VPROG. Due to the multiple vernalisation completion criteria, the predicted anthesis date is unaltered when these parameter values are explored individually. If VPROG is altered by changing VAI or VBEE or LF_{max}, vernalisation can still be fulfilled within a time frame that does not influence modelled output (anthesis date). As a result, if values of VAI, VBEE and LF_{max} are individually explored, no effect is seen. However, if VAI and VBEE are both set to 0 (no vernalisation requirement), or VBEE alone is set to 0, a substantial effect is noted. For example, Alchemy flowered 45 days earlier if both these parameters with set to zero. The variability in VAI estimates, and the highly significant correlation with VBEE ($p<0.001$) support the conclusion reached by He et al. (2012), that there is a compensation phenomenon occurring between these two parameters describing aspects of the vernalisation process.

Table 3.5 Correlation matrix for cultivar parameters generated during parameterisation of 16 cultivars for Sutton Bonington (UK), Clermont-Ferrand (France) and Estrees-Mons (France). *p<0.05, **p<0.01, ***p<0.001. The matrix was generated using accepted parameter values during calculation of the best fitting parameterisation for the 16 cultivars.

	LF_{min}	LF_{max}	A_{max}	EXTINC	PHYLL	SLDL	TTANBGF	TTBGEG	TTSOWEM	VAI	VBEE
LF_{min}	1.00										
LF_{max}	0.17***	1.00									
A_{max}	-0.11**	0.43***	1.00								
EXTINC	0.11**	0.07	0.24***	1.00							
PHYLL	-0.66***	-0.43***	-0.39***	-0.13***	1.00						
SLDL	-0.12***	0.36***	0.76***	0.17***	-0.50***	1.00					
TTANBGF	0.01	-0.11**	-0.32***	-0.30***	0.25***	-0.41***	1.00				
TTBGEG	-0.27***	-0.01	-0.07	0.01	-0.03	0.18***	-0.12**	1.00			
TTSOWEM	0.15***	0.38***	-0.13***	-0.15***	-0.28***	-0.15***	0.13***	0.11**	1.00		
VAI	-0.18***	0.36***	0.71***	-0.03	-0.34***	0.72***	-0.36***	0.12***	-0.03	1.00	
VBEE	0.05	0.50***	0.81***	0.07	-0.48***	0.77***	-0.39***	-0.08*	-0.11**	0.73***	1.00

3.3.3 Model Reduction

3.3.3.1 Variables

The potential for reduction of the Sirius model was assessed using the best fit parameterisations produced for the 16 cultivars. In this analysis (described in Section 2.8), model variables are assessed for potential redundancy. Numerous model formulations are generated, each based on the full model but with certain variables replaced by fitted constant values. The effect of replacing a model variable with a fitted constant on the model's predictive performance is assessed, with the expectation that replacing a variable that was important for model prediction with a fixed constant would have a detrimental effect on the model's predictive performance. Although not explicitly performed here, previous Sirius model reduction analysis has demonstrated that application of the model with redundant variables replaced with fitted constants produces similar simulations of total and biomass to the full model, and improved simulation of grain biomass and leaf area index (Crout et al., 2014).

The reduction analysis was conducted in two stages; an initial screening analysis, and a more comprehensive multi-factorial analysis. Initially, all model variables with the exception of those providing diagnostics or outputs were considered.

The screening analysis identified 67 model variables that could be replaced by a constant, without resulting in model failure. For the majority of these variables, their individual replacement with a constant either resulted in a large increase in the Residual Sums of Squares (>50%), or caused a reduction in SS_{res} (Figure 3.10). Only variables which had produced a smaller SS_{res}, or a small increase in SS_{res} (<10%) were considered for inclusion in the multi-factorial analysis. 22 variables

increased the ratio of SS_{res} for the reduced model to the SS_{res} for the full model to more than 1.1, and therefore were discarded from the subsequent analysis. The remaining 45 variables were considered as candidates for redundancy.

Due to the computational expense of the multi-factorial analysis, before conducting the multi-factorial analysis, a mechanistic assessment of the variables role in the model was performed. Intermediate variables whose reduction could be better performed by replacing the end variable, and those variables that would result in the simulation of inappropriate or uncontrolled processes were discarded. For example, variable replacement that would break the mass balance of the model. On this basis, 14 variables remained and were including in the multi-factorial analysis, alongside an additional five 'switch' variables. As in the analysis performed by Crout et al. (2014), these variables 'switched off' processes within the model for which candidate redundant variables had been identified.

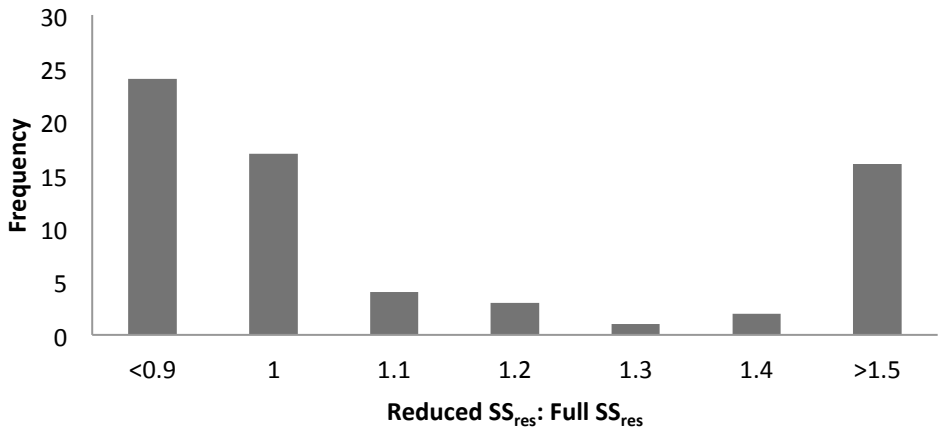


Figure 3.10 Frequency of the ratio of the reduced model residual sum of squares (Reduced SS_{res}) to the full model (Full SS_{res}) for the 67 variables considered in the screening analysis.

The multi-factorial analysis was assessed by parameter replacement probabilities (R_p). The value of the replacement probability indicated the effect of the variable replacement on model performance, with values tending to zero indicating that model performance was worsened with variable replacement, and values tending to one implying that performance was improved. A value of 0.5 implied that model performance was indifferent to the variable replacement and suggested that the variable was redundant. Graphical analysis ensured that relatively stable replacement probability values were produced during the multi-factorial analysis (Figure 3.11).

The results of the multi-factorial analysis are summarised in Table 3.6. Variables describing temperature adjustments, grain filling, nitrogen mineralisation, evaporation, leaf expansion and vernalisation were included in the analysis.

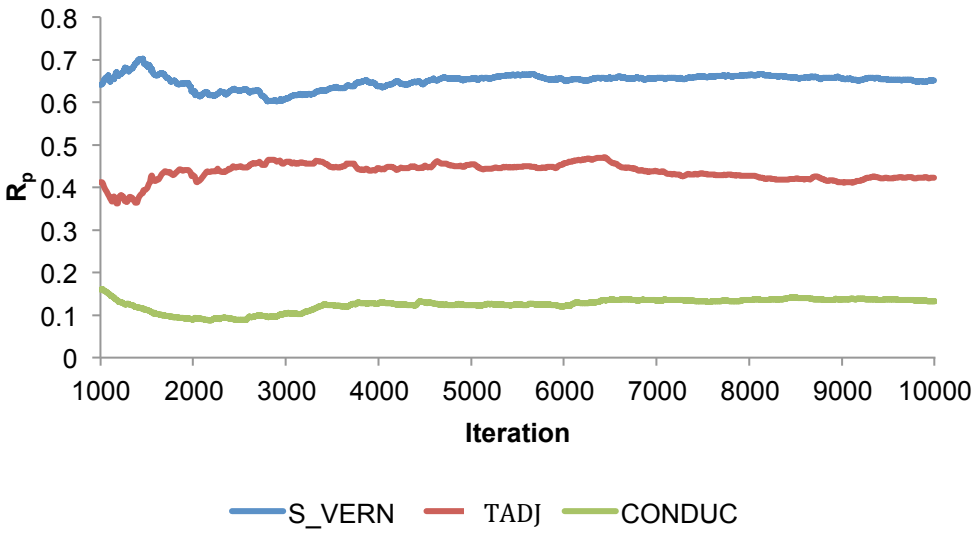


Figure 3.11 Replacement probability (R_p) evolution for candidate variables S_VERN (vernalisation switch), TADJ (temperature adjustment: soil) and CONDUC (temperature adjustment: canopy) during the multi-factorial analysis.

Switch variables describing the removal of air temperature adjustments had low replacement probabilities, indicating that simulating differences between air, soil and canopy temperatures contributed to model predictive power. Two other variables involved in adjusting temperatures within the model – ENAV and CONDUC – were also identified as contributing to model predictions, although a third – TADJ – was borderline redundant.

Biomass at anthesis (BIOANTH) was assessed as being redundant (R_p=0.54), as were the variables describing the influence of temperature (TA) and moisture (F_m) on the rate of soil mineralisation. A variable involved in the calculation of soil surface evaporation (ALPHA, R_p=0.57) was also indicated to be redundant, with variables describing the effect of drought on canopy senescence (GAKILR) and expansion (SF) identified as borderline redundant (R_p=0.42) and improving model predictive ability (R_p=0.34), respectively.

The variable SF, representing the ration of actual to potential transpiration is used in the determination of the effect of drought on canopy sensence (GAKILR). In the simulations, this effect was only present at one site (Clermont-Ferrand) for one season. Removal of this effect from the simulation had a negligible effect on estimated final biomass, yield and LAI.

The evaporation variables EW, WND and A_SUM were assessed as redundant in this analysis, with HSLOP_TMEAN identified as borderline redundant. Although one variable involved in the calculation of vernalisation was identified as improving model predictive ability (R_p=0.36) when this process was simulated, the analysis indicated that model performance could be improved if this process was switched off (S_VERN, R_p=0.65).

In the analysis of vernalisation variables, it was indicated that, if this process was simulated (S_VERN=1), only one variable was identified as contributing to model predictions (PRIMORDNO). Other assessed variables (e.g. POTLFNO), were assessed as redundant by the analysis, and further investigation demonstrated that the conditions under which this variable would be utilised were not met. This variable is used to end the process of vernalisation when the primordia number (PRIMORDNO) exceeds the potential number of leaves (POTLFNO), to prevent later sowing producing early maturity. Although PRIMORDNO is used in the recalculation of LF_{min}, which in turn is used in the determination of final leaf number (FLN), POTLFNO has no other impact within the model.

The redundancy identified by the analysis, suggested that the effect of temperature on soil mineralisation (TA) could be effectively replaced by using a constant soil temperature of 15.54°C, resulting in the effect of temperature on soil nitrogen mineralisation being represented by a constant value of 1.7. The effect of moisture on soil mineralisation (F_m) could also be described by a constant value, rather than being a function of soil water.

Analysis of the modelled processes demonstrated that the redundancy of the evaporation variables HSLOP_TMEAN, A_SUM, EW, WND and ALPHA and replacement with constants, resulted in simulation of evapotranspiration being based upon interception of radiation by the canopy, with the removal of the effects of wind, saturated vapour pressure and the temperature, resulting in a further simplification of the Priestley-Taylor equation.

In the previous analysis of Sirius for variable redundancy, Crout et al. (2014) identified 16 potentially redundant variables. Considerably fewer potentially

redundant variables were identified in this analysis, with only six variables - describing carbon translocation, soil mineralisation, evaporation and vernalisation - being identified as redundant. Although some variables were identified as redundant in both analyses, for example BIOANTH, S_VERN, TA and F_m, there were also a number of conflicting results. In this analysis, the temperature adjustments were important in maintaining model predictive ability, but they were largely found to be redundant by Crout et al. (2014). Additionally, were variables were replaced with constant values, significant differences in values were noted between the two analyses. For example, both the models identified that temperature and moisture effects on nitrogen mineralisation could be described by constant values, but the previous study estimated values at the low end of the range for these new constants (5.58 and 0.39, respectively), whilst here they were fitted with values at the higher end of the range (16 and 1, respectively). Similarly for evapotranspiration, both in the sensitivity analysis performed by Brooks et al., (2001) and the model reduction by Crout et al. (2014), much lower values for constants applied for estimating evapotranspiration were determined.

Two variables describing nitrogen uptake were identified as redundant in the previous analysis (Crout et al., 2014), but did not pass the screening stage here (SS_{res} ratio >1,1), indicating their importance in maintaining model predictive power. Although the process of vernalisation was identified as redundant in both these analyses, two vernalisation variables were also identified as redundant previously (Crout et al., 2014), whilst here, only one was included in the analysis, and was found to improve model performance when the process was simulated (R_p=0.36).

Table 3.6 Candidate variables considered in the multi-factorial analysis.

Model Variable	Function	Min.	Max.	Replacement Constant	Replacement Probability
Temperature Adjustments					
S_CTEMP	Switch to set canopy temperature to air temperature	-	-	0	0.01
S_SOILMAX	Switch to set the estimate of soil temperature maximum air temperature. Maximum soil temperature is used in the early stages of growth to estimate the temperature controlling plant processes	-	-	0	0.30
S_SOILMIN	Switch to set the estimate of minimum soil temperature to minimum air temperature. Minimum soil temperature is used in the early stages of growth to estimate the temperature controlling plant processes.	-	-	0	0.31
S_HTEMP	Switch to remove the diurnal temperature adjustments	-	-	0	0.32
ENAV	A soil heat physics calculation, influencing the calculation of canopy temperature and maximum soil temperature	-0.09	17.33	2.37	0.26
CONDUC	Denominator in the correction applied to air temperature to estimate canopy temperature	0.91	8.86	1.9	0.13
TADJ	Temperature correction based on mean air temperature, which influences the calculation of maximum soil temperature	0	8.35	0.56	0.42
Grain filling					
BIOANTH	Biomass at anthesis. Used to determine the maximum biomass available for translocation during grain filling.	5100	10495	7304	0.54
Nitrogen mineralisation					
F_m	Factor representing the influence of soil moisture on nitrogen mineralisation	0.26	1	1	0.51
TA	7-day moving average air temperature, used to calculate the effect of temperature on nitrogen mineralisation	-4.26	22.76	16	0.52
Soil surface evaporation					
ALPHA	Factor representing the effect of canopy shading on soil surface evaporation	1	1.35	1.24	0.61
Leaf Expansion					

Model Variable	Function	Min.	Max.	Replacement Constant	Replacement Probability
GAKILR	Factor used to represent the effect of drought on canopy senescence	0	1.7	0.99	0.42
SF	Factor representing the effect of drought on canopy expansion, (also used to calculate effect of drought on biomass growth and nitrogen availability)	0.22	1	1	0.34
Evaporation					
A_SUM	Intermediate variable used in the calculation of vapour pressure deficit, used in the calculation of evaporation	0.028	0.025	0.034	0.48
EW	Intermediate variable used in the calculation of vapour pressure deficit, used in the calculation of evaporation	3.17	33.41	18.78	0.62
HSLOP_TMEAN	Intermediate variable used in calculation of Priestly-Taylor evaporation	0.25	1.93	1.05	0.41
WND	Wind speed, used in the calculation of Penman evaporation (from Priestly-Taylor evaporation)	0	11.3	2.51	0.52
Vernalisation					
S_VERN	Switch to remove the influence of vernalisation on crop development	-	-	0	0.65
PRIMORDNO	Primordia number, used in the calculation of vernalisation effect on crop development	4	17.15	10.57	0.36

3.3.3.2 Parameters

In addition to the model variables considered here and in the previous model reduction analysis of Sirius, the observations for multiple cultivars in the dataset facilitated the assessment of the cultivar-specific parameters themselves for redundancy. For this analysis, the cultivar-specific parameters were re-assigned as variables, which enabled replacement of these cultivar-specific values with a generic constant to describe growth and development.

Parameters describing absolute minimum leaf number (LFmin), photoperiod response (SLDL) and phyllochron (PHYLL) were not included in the multi-factorial analysis (SS_{res} ratio>1.1) as they were discarded at the screening analysis. The

remaining parameters included in the multi-factorial analysis were the two parameters describing vernalisation rate (VAI and VBEE), maximum potential leaf area (A_{max}), thermal time from sowing to emergence (TTSOWEM), thermal time from anthesis to the beginning of grain-fill (TTANBGF), thermal time from the beginning of grain-fill to the end of grain-fill (TTBGEG), absolute maximum leaf number (LF_{max}) and the extinction coefficient (K_e) (Table 3.7).

Table 3.7 Cultivar parameters re-assigned and considered candidate variables in the multi-factorial analysis. listed in order of replacement probability, smallest to largest.

Model Variable	Function	Min.	Max.	Replacement Constant	Replacement Probability
TTSOWEM	Thermal time duration of the period from sowing to emergence	100	250	224	0.22
TTANBGF	Thermal time duration of the period from anthesis to the beginning grainfill	50	144	61	0.50
TTBGEG	Thermal time duration of the period from beginning of grainfill to the end of grainfill	400	650	506	0.55
LF_{max}	Absolute maximum leaf number	13.8	27.9	21.4	0.55
VBEE	Vernalisation rate	0.004	0.067	0.036	0.50
VAI	Response of vernalisation rate to temperature	0	0.01	0.005	0.49
A_{max}	Maximum potential area of each leaf layer	0.002	0.003	0.003	0.58
K_e	Extinction coefficient of the crop canopy	0.36	0.62	0.52	0.63

Of the cultivar parameters included in the multi-factorial analysis, all but TTSOWEM were identified as redundant by the analysis (Table 4.6). This analysis indicates that all parameters considered cultivar-specific outside of the phenology sub-model (A_{max}, TTBGEG, TTANBGF, and K_e), are redundant, and implied that the ability to predict

differences in cultivars could be maintained by the model by only estimating cultivar-specific values for TTSOWEM, PHYLL, SLDL and LF_{min}. In effect, cultivar differences can be modelled using Sirius by considering only thermal time between sowing and emergence, leaf emergence rate, and photoperiod response.

LF_{max} was assessed as redundant in this analysis. This was unsurprising, as its function in the model is to act to prevent late sowing resulting in early maturity, an event that was not present in the trial dataset.

Further analysis revealed that the description of vernalisation could be described by replacing the cultivar parameters VBEE and VAI with constants, which resulted in the progression of vernalisation being described by constant accumulation of 0.036 and 0.074 per day, for temperatures in the range 0-12°C and 13-17°C, respectively. This replacement of cultivar-specific vernalisation parameters with constants, suggested that differences in cultivar vernalisation response are being described / captured by alternative parameters in the model. Analysis of the simulation revealed that despite the potential of VAI and VBEE to affect the progress of vernalisation, the final leaf number was being set by primarily by the LF_{min} parameter, with this value was used to calculate the final number of leaves (FLN), effectively removing the effect of vernalisation. However, for cultivars with a low estimated LF_{min} (e.g. Arche), the FLN could be determined using the PRIMORDNO, although this only occurred rarely (for Arche, only once over the 12 site-year-nitrogen simulations).

In an earlier analysis of the sensitivity of Sirius to cultivar parameters, it was also noted that the model was sensitive to minimum leaf number (LF_{min}), and that the high values assigned to this meant that the process of vernalisation (and therefore the vernalisation parameters, VAI and VBEE) had no effect on final leaf number (Brooks

et al., 2001). Consequently, either minimum leaf number or vernalisation variables would be important in model predictive ability, dependent on the (value fitted to minimum leaf number for the) cultivar. This effect was also noted in this analysis.

Similarly, analysis of the TTANBFG and TTBGEG parameters, revealed that whilst these were being utilised to control processes in the model, i.e. controlling the switching between phases rather than, for example, the absence of any LAI in the instance of TTBGEGB, constant values were sufficient and any differences in cultivars could be described using other parameters.

A previous analysis of Sirius cultivar-specific parameters considering their correlations within the phenology sub-model, concluded only three parameters were required to describe cultivar differences in anthesis date – SLDL, VAI and PHYLL (He et al., 2012). Although SLDL and PHYLL were considered important for model anthesis date predictions here, the process of vernalisation and its associated parameters were not. However, He et al. (2012) did observe that the model was more sensitive to SLDL than the vernalisation parameters, as was demonstrated in the analyses here. Additionally, He et al. (2012) removed TTSOWEM from the parameterisation due to its relatively high level of interactions with other parameters and low sensitivity index. In this analysis, TTSOWEM was the only parameter that was significantly correlated with all other estimated parameters, all but one at a highly significant level ($p<0.001$), although, on average across the values explored, the model was less sensitive to six other cultivar-specific parameters.

3.4 Conclusions

Overall, the results indicated that that model is over-parameterised, as a result of the inability to obtain a robust parameterisation for cultivars – the parameter estimate

was affected by the selection of initiating value, could not be guided by informed prior distributions and their were a large number of significant inter-correlations between the parameters being. Therefore multiple rounds of estimation were used to identify the best fit for each cultivar. Using a different approach focused on the phenology sub-model, the same conclusion was reached by He et al. (2012).

The reduction analysis expanded on previous work, to include a dataset describing a larger number of cultivars, which contained cultivars with a broad range of vernalisation response, daylength sensitivity and observed flowering dates. The analysis indicated that there are redundant variables within the Sirius model, similarly to the previous investigation, although only a relatively small number of model variables were identified (Crout et al., 2014). Most of the model variables were identified as not redundant. In total, only six variables - describing carbon translocation, soil mineralisation, evaporation and vernalisation - were identified as potentially redundant. This was considerably fewer than the previous analysis, which identified 16 variables in total, with the additional redundant variables describing nitrogen uptake, vernalisation, evaporation and temperature adjustments. Despite the observations including a relatively large number of cultivars, with a broad range of vernalisation responses, switching off the vernalisation process in the model was still identified as improving model predictions.

A sensitivity analysis of the model outputs to cultivar-specific parameters suggested the model was most sensitive to changes in the values of parameters describing the phyllochron (PHYLL), photoperiod response (SLDL) and absolute minimum leaf number (LF_{min}). Insensitivity was demonstrated to a number of parameters involved in the calculation of vernalisation. Similar results were noted by Brooks et al. (2001).

As expected for a complex, mechanistic model, there are a large number of highly significant parameter correlations ($p<0.001$). As the sensitivity analysis assumes parameter independence, a model reduction focused on the cultivar-specific parameters was performed in support of the sensitivity analysis. This indicated that of the 11 parameters, only four were required to maintain model predictive power (TTSOWEM, PHYLL, SLDL, LF_{min}). Thus the model reduction analysis supports the results of the sensitivity analysis, confirming the insensitivity of the model to the vernalisation parameters, which were identified as redundant, with their replacement with constant, non-zero values, not affecting model predictive ability.

A major limitation of the reduction analysis is the mechanistic interpretation by the researcher prior to the multi-factorial analysis and the dependence on the observational data used. In the analysis performed by Crout et al. (2014), the datasets included detailed growth analysis for two cultivars under both potential and water and nitrogen limiting conditions in the UK and New Zealand. Here, the observations were less detailed and considered only potential and nitrogen limiting conditions, but with a larger number of cultivars. Therefore, it is not unexpected that certain variables are identified as less important to model predictions in this analysis, for example those describing drought effects. In contrast, the larger number of nitrogen-limited and potential treatments observations resulted in the exclusion of nitrogen uptake variables previously identified as redundant from this analysis. The results of these reduction analyses are a property of/limited by the data used. Neither analysis provides a full assessment of all modelled processes, and so must be considered partial (Crout et al., 2014). The areas identified as redundant are those that are redundant for the data used in the analysis (i.e in the application in this thesis; describing the leaf area, biomass and yield of multiple cultivars under

variable nitrogen treatments) – it does not follow that they will be redundant in other applications of the model. This has been demonstrated here, for example, for variables describing nitrogen uptake, despite nitrogen treatments datasets being utilised in both reduction exercises. Even where there were consistently identified areas of redundancy within the model, for example, the effects of temperature and moisture on soil mineralisation, very different values were fitted for the replacement constants.

Additionally, although this analysis indicates that these processes, and the variables within them, may be redundant in the model of the system, it does not follow that they are redundant in the real system. It might be that the modelled process is not close enough to reality to be useful. For example, vernalisation, whilst clearly having an important effect on phenology in real wheat plants, does not appear to be necessary in this application of the model.

The complexity demonstrated by the results of the analyses demonstrate that the results of simple sensitivity analyses and parameterisations need to be very cautiously interpreted, although the reduction analysis provides important support to the sensitivity analysis, it is subject to its own limitations.

Given the results of the reduction analyses, it could be argued that a model of lesser complexity could be more appropriate. Such a model could still aim to simulate differences in cultivar growth and development, but do so utilising fewer processes, and subsequently a smaller number of parameters and variables. Thus, a model of intermediate complexity could be developed, removing or reducing the parameters and descriptions identified here, by Brooks et al., (2001), by He et al. (2012) and by Crout et al. (2014) as being potentially redundant.

4 A New Mechanistic Model of Intermediate Complexity: Field-Scale

4.1 Introduction

In the previous chapter (Chapter 3), a comprehensive model reduction method was applied to the existing mechanistic model, Sirius. This assessed the model for processes and parameters that are redundant, i.e. do not contribute to model predictive ability, when describing the performance of 16 cultivars over limiting and non-limiting nitrogen regimes. A number of processes and parameters were found to be redundant, in line with previous assessments of this model, and a reduced version of Sirius, Sirius-R, was produced (Brooks et al., 2001; Crout et al., 2014).

Given these results of the reduction analyses, it could be argued that a model of lesser complexity could be more appropriate. Such a model could still aim to simulate differences in cultivar growth and development, but do so utilising fewer processes, and subsequently a smaller number of parameters and variables, thus potentially being more applicable where input and calibration data is less available, or at differing scales – for example, to predict yields at the farm level.

In particular, simplifying the simulation of phenology, by no longer considering individual leaf formation and development, and therefore reconsidering the simulation of LAI and vernalisation effects, which were identified as the greatest source of predictive error and being potentially redundant, respectively in the previous analysis (Chapter 3).

simplifying the simulation of phenology, by no longer considering individual leaf formation and development, and therefore reconsidering the simulation of LAI and vernalisation effects, which were identified here as the greatest source of predictive error and being potentially redundant, respectively.

4.1.1 Aims

Considering the above, the aims of this chapter are to:

- To develop, parameterise and analyse for reduction, a mechanistic model of intermediate complexity using field level observations
- Assess the ability of this intermediate model to simulate differences in cultivar growth and development, relative to the Sirius model
- Investigate the application of this intermediate model to farm-level yield prediction

4.2 Model Description

The intermediate model simulates nutrient-limited canopy, biomass and grain growth on a daily time-step as a function of available soil water and nitrogen, as well as basic phenology, using the parameters in Table 4.1 to describe differences in cultivar phenology.

Table 4.1 Model parameters describing crop growth and development.

Parameter	Description	Constraints
Canopy		
LAI_0	Canopy size (°Cd)	2760 - 10396
LAI_μ	Canopy timing (°Cd)	n/a
LAI_σ	Canopy duration (°Cd)	n/a
Biomass		
RUE	Radiation use efficiency (g MJ^{-1})	1.2 – 2.5
K_e	Extinction coefficient	0.45 – 0.70
Phenology		
TTSOWEM	Thermal time from sowing to emergence (°Cd)	
TTFLIN	Thermal time from emergence to floral initiation (°Cd)	150 – 175
TTANTH	Thermal time from emergence to anthesis °Cd)	300 - 500
TTANBGF	Thermal time from anthesis to grain fill initiation °Cd)	900 - 1300
TTBGEG	Thermal time from grain fill initiation to end (°Cd)	50 – 160
P1D	Photoperiod sensitivity	0 – 65
P1V	Vernalisation requirement (days)	0 – 30

4.2.1 Phenology

A basic consideration of phenology is simulated, controlled by thermal time parameters. As thermal time accumulates, the crop progresses through four thermal time phases;

(i) thermal time from sowing to emergence (TTSOWEM)

(ii) thermal time from emergence to anthesis (TTANTH)

(iii) thermal time from anthesis to grain fill initiation (TTANBGF)

(iv) thermal time from grain initiation to end (TTBGEG)

An additional thermal time parameter, TTFLIN, is also required to control the application of vernalisation and photoperiod effects.

4.2.2 Vernalisation & Photoperiod

The vernalisation response of cultivars is estimated using a factor altering the accumulation of thermal time as described by McMaster et al. (2008), a version of which is incorporated in the complex, mechanistic model, APSIM (Keating et al., 2003).

$$F_{V\,zero} = 1 - \frac{P1V}{50} \qquad \textbf{Equation 4.1}$$

$$F_V = F_{v\,zero} + \frac{\sum Vdays}{P1V} \qquad 0 \leq F_V \geq 1 \qquad \textbf{Equation 4.2}$$

Where $F_{V\,zero}$ is the un-vernalised development rate, F_v is the vernalisation factor, P1V Is the parameter describing photoperiod sensitivity, and Vdays is the number of accumulated vernalising days.

The daily photoperiod (PP) is calculated as in Sirius, but the response of cultivars is estimated in a manner similar to the vernalisation response (McMaster et al., 2008).

$$F_D = 1 - \left[\frac{P1D}{10000}(20 - PP)^2\right] \qquad 0 \leq F_D \geq 1 \qquad \textbf{Equation 4.3}$$

Where F_D is the daylength or photoperiod factor and P1D is the cultivar sensitivity to photoperiod.

Accumulated thermal time (TT), in the relevant growth stages, is then calculated as:

$$TT = TT + \Delta TT \min(F_D, F_V)$$ **Equation 4.4**

Where ΔTT is the change in thermal time. No temperature adjustments for soil, canopy and diurnal temperature differences are included in this model.

4.2.3 Canopy

Canopy leaf area index (LAI) was not well simulated by Sirius in the analysis performed by Crout et al. (2014), with improved simulation noted using the reduced form of the model. In the intermediate model, a much simpler description is used, based on a modified form of the model of Gillett et al. (1999). This was incorporated in a differential form, to allow nitrogen and water availability to directly impact on leaf area index (LAI) growth at each time-step.

$$\frac{\Delta L_{pot}}{\Delta TT} = \frac{LAI_0}{2.51 LAI\sigma} * LAI\mu - TT \frac{1}{LAI\sigma^2} * e - 0.5(\frac{LAI\mu - TT}{LAI\sigma})^2$$ **Equation 4.5**

Where L_{pot} is the potential increase in LAI, LAI_0 describes the size of the canopy, LAI_μ describes the timing of the canopy and LAI_σ describes the duration of the canopy.

For each time-step, the potential increase in LAI can be restricted first by nitrogen, and then by water availability to determine the nutrient-limited increase in LAI (ΔL_{actual}):

$$\Delta L_{actual} = \Delta L_{pot} * Nf * Sf \qquad 0 \leq Nf \geq 1 \qquad 0 \leq Sf \geq 1$$ **Equation 4.6**

Where N_f is the ratio between plant available nitrogen and nitrogen required for potential growth (4.2.6), and S_f is the ratio between actual and potential evapotranspiration (4.2.7).

4.2.4 Biomass

Biomass growth is related to solar radiation and temperature using the classical model of light interception and conversion (Monteith, 1969). Prior to the start of grain growth, after the demand for leaf biomass is satisfied, any remaining biomass is assigned to the stem. After anthesis, all new biomass is assigned to the grain.

4.2.5 Plant Nitrogen

Plant nitrogen dynamics are simulated using descriptions from Sirius. Prior to anthesis, after the leaf demands for nitrogen are met, any remaining nitrogen is assigned to the stem. Leaf and stem nitrogen demands are controlled using the parameters SLN and $maxS_N$ (Equation 4.7). After the nitrogen required for leaf growth (L_{actual}) has been removed from that available, any additional nitrogen is assigned to the stem, which is able to 'store' excess nitrogen up to a maximum defined by the parameter $maxS_N$ (Equation 4.8).

$$\boldsymbol{L_N = L_{actual} * SLN}$$ **Equation 4.7**

$$\boldsymbol{S_N = B_S * (maxS_N - (T_N - L_N)}$$ **Equation 4.8**

Where L_N is the nitrogen required for the increase (L_{actual}) in leaf area growth,

determined using the Specific Leaf Nitrogen (SLN, kg N m^{-2}). S_N is the increase in stem nitrogen (kg N m^{-2}), T_N is the total available nitrogen (kg N m^{-2}), maxS_N is the maximum stem nitrogen (kg N kg^{-1} DM) and B_S is the increase in stem biomass (kg m^{-2}).

This allows the stem to uptake nitrogen exceeding current crop demand from the soil, with this excess available to supplement plant nitrogen requirements if necessary in the future. During canopy senescence, nitrogen from senesced leaf area is relocated to the stem, with only a small structural element unavailable.

After anthesis, the stem provides a pool of nitrogen for grain growth (S_{exN}), with nitrogen available to remobilised above a critical minimum value, minS_N (kg N kg^{-1} DM) (Equation 4.9).

$$S_{exN} = S_N - (minS_N * S_B) \qquad \textbf{Equation 4.9}$$

Where S_B is the current stem biomass (kg m^{-2}).

Although uptake of additional nitrogen from the soil is permitted, this ability is gradually reduced as grain-fill progresses (Equation 4.10). If there is insufficient nitrogen available from these sources, then the deficit is met by prematurely senescing leaf area.

$$G_f = \frac{\text{TTBGEG} - TT_{GF}}{\text{TTBGEG}} \qquad 0 \leq Gf \geq 1 \qquad \textbf{Equation 4.10}$$

Where G_f is the fraction of available nitrogen that the plant is permitted to uptake, TT_{GF} is the thermal time since grainfill start (°Cd) and TTBGEG (°Cd) is a parameter describing thermal time from grain fill initiation to end.

4.2.6 Soil Water and Nitrogen

The soil profile is considered to be one layer, over which resources (i.e. nitrogen and water) are evenly distributed. Rainfall and nitrogen fertiliser applications are immediately added to, and evenly distributed throughout, this profile. The soil profile depth is 1.50 m, based on observations of wheat root depth, as in Sirius (White et al., 2015).

Many of the descriptions of soil water and nitrogen dynamics are based on those in Sirius. Three soil moisture parameters describe the soil characteristics controlling water and nitrogen dynamics; (i) drained upper limit (S_{DUL}), (ii) lower limit (S_{LL}) and (iii) saturation (S_{SAT}). Soil water is split into three categories, depending on its availability for uptake by the crop; excess, available and unavailable. Water below S_{LL} is unavailable, water above S_{DUL} is excess and readily available, and water held between these limits is available to the crop, although limited by a maximum daily extraction amount. This extraction limit is estimated to be 10% of the available soil water, a simplification of an extraction function used in Sirius. Water is percolated into the available water bucket first, followed by the excess water bucket, up to a maximum level as determined by S_{SAT}. All further water is immediately lost.

Soil nitrogen is associated with the soil water, with nitrogen split proportionally between unavailable and available water. Nitrogen equilibrates over time between the available and unavailable water, at a rate of 40% per day. Nitrogen is assumed to not be held in excess water. A small quantity of nitrogen (5%) is lost to denitrification upon application and organic soil nitrogen is mineralised as a function of average weekly temperature and soil moisture.

Plant available water and nitrogen are a function of the rooting depth, with the growth of roots simulated as a function of thermal time, assumed to grow directly downwards through the soil profile, with root length equal to root depth. Root growth ceases at anthesis. The fraction of plant available soil water and nitrogen that can be captured by the crop is calculated as a function of root length (RL) and soil profile depth (D) (Equation 4.11). Plant nitrogen uptake is restricted to a maximum of 5 kg ha^{-1} day^{-1}, as in Sirius.

$$F_{capture} = RL/D \qquad \textbf{Equation 4.11}$$

4.2.7 Evapotranspiration

Potential soil evaporation and transpiration are calculated using the two-stage evaporation model (Ritchie, 1972), using the Priestley-Taylor equation to remove reliance on additional meteorological observations. Evaporation and/or plant water uptake is restricted if the quantity of water available in the profile does not meet requirements for potential evaporation and/or transpiration. Determination of water available for plant uptake is described above. Water available for evaporation from the soil profile is that held in the upper 25cm, a simplification of the multi-layered description in Sirius. In this simplified model, the water is considered evenly distributed, and the quantity available for evaporation is:

$$EVAP_{POT} = (0.25)/D * W \qquad \textbf{Equation 4.12}$$

Where $EVAP_{pot}$ is the water available for evaporation, D is the depth of the soil profile and W is the water in the soil profile.

4.3 Results and Discussion

4.3.1 Field Scale

4.3.1.1 Model Development

Initially, two datasets were employed to assess the model's ability to simulate the effects of nitrogen and water availability on leaf area, biomass and yield. Nitrogen trial data from Sutton Bonington (SB) and rain shelter trial data from Lincoln were selected. This also allowed the simulation of both spring (Lincoln) and winter (SB) wheat, as well as wheat growth and development under both nitrogen and water non-limiting and limiting environments.

The model was parameterised for both datasets using constraints guided by a range of previously determined values for wheat cultivars in Sirius and APSIM. Soil parameters used were determined for the two sites in previous work (Gillett et al., 1999).

The model was better able to simulate the effects of nitrogen dynamics on grain yield, biomass and LAI, than drought. It was especially poor at simulating the effects of drought on LAI (Figure 4.1, wMAPE = 51%). Although it produced much better simulations of yield and biomass across the four rain shelter treatments (Figure 4.2 & Figure 4.3, wMAPE = 21% & 16%, respectively), it under-estimated both at the highest irrigation level. Analysis of the simulation revealed that although no water stress was experienced by the wheat under this scenario, nitrogen stress was experienced during grain filling preventing the attainment of potential yield and biomass. Actual growth was restricted to an average of 84% of potential over a seven-day period.

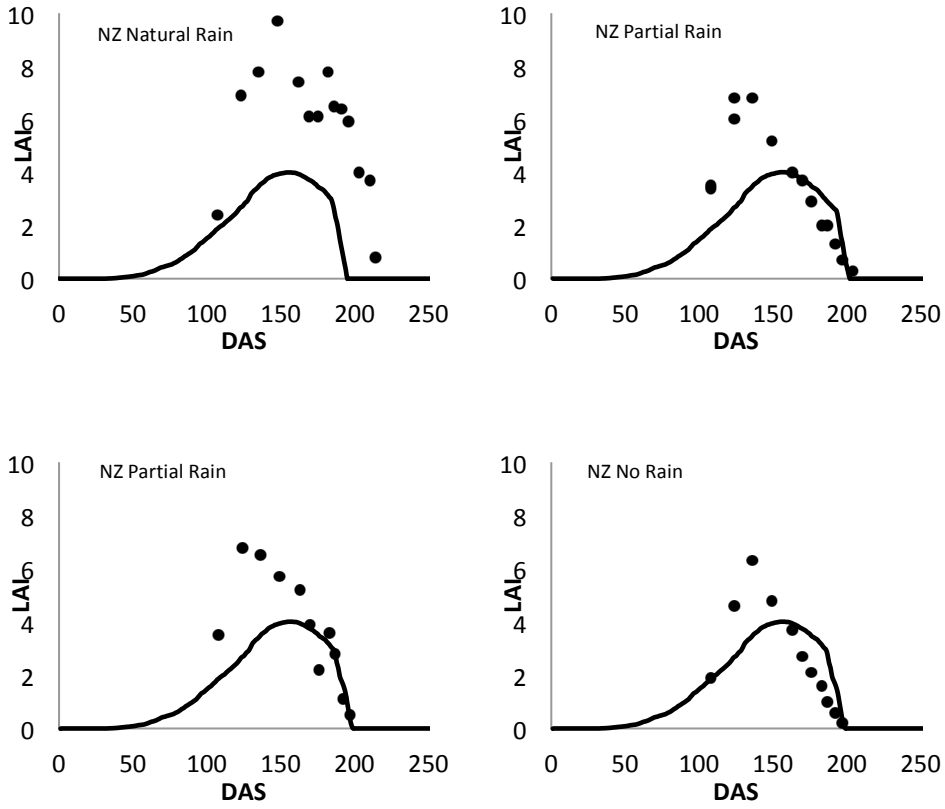


Figure 4.1 Time series of simulated (-) and observed (x) LAI. Weighted Mean Absolute Percentage Error (wMAPE) of 51%

Despite the reduced LAI simulated, the model was still able to simulate total and grain biomass well. In the simulation, LAI was 'averaged out' when the model was parameterised for the rain shelter trials, with all four treatments simulating a peak LAI of approximately 4, whilst the observed LAI values ranged from 6 to 10 (Figure 4.1). This indicates that variation in the LAI was not important in simulating variation in the total and grain biomass. In Figure 4.1, it can be noted that the slower growth of the LAI results in a delay in reaching the peak LAI value for three of the four treatments. This delay, resulting in the peak fractional interception occurring later in the growing

season, reduces the importance of canopy size in achieving the simulated total and grain biomass.

Within the model, a parameter, Specific Leaf Weight (SLW, 0.045 kg m^{-2}), is used in the determination of the required biomass for leaf area growth. The leaf area increase is not limited by the biomass increase available, however, so there is the potential that an implausible crop could be simulated with excessively thin leaves. Analysis of the values here did not indicate that this was the case in this instance. A Specific Leaf Area (SLA, m^2 kg^{-1}) of approximately 22 m^2 kg^{-1}, equivalent to a SLW of approximately 0.045 kg m^{-2} was maintained throughout the simulation.

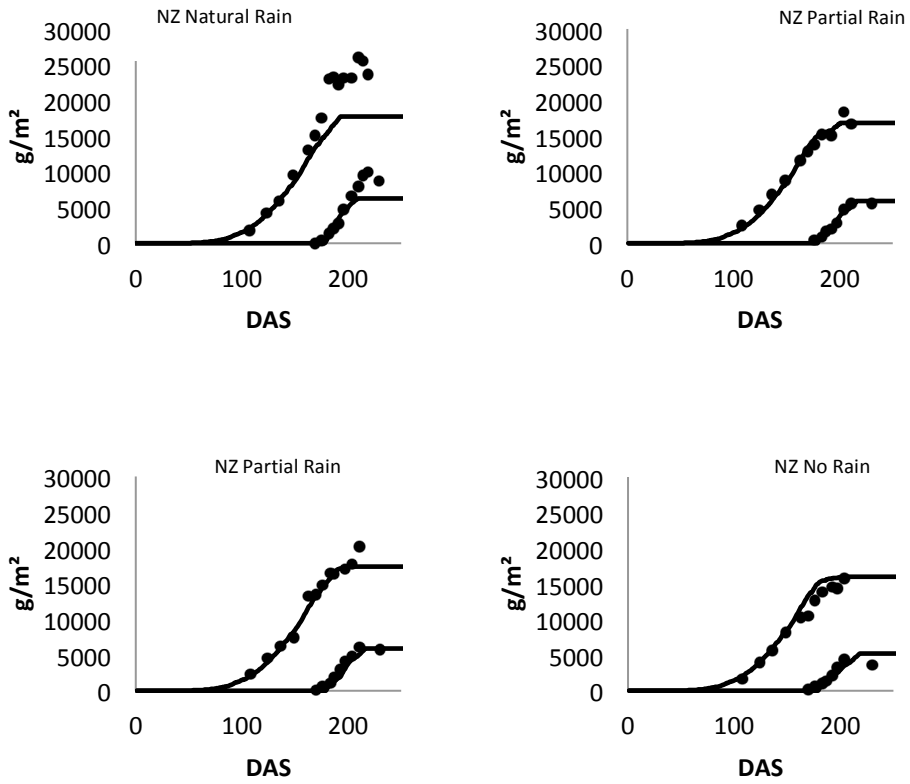


Figure 4.2 Time series of simulated (-) and observed (x) total and grain biomass (g/m^2). Grain biomass values are in the bottom right of all graphs. Weighted Mean Absolute Percentage Error (wMAPE) of 16% and 21% for total and grain biomass, respectively.

Similarly, when simulating the low nitrogen treatment at SB (Figure 4.3), a small increase in modelled LAI can be seen during senescence. This is the result of a fertiliser application, during a period where the potential leaf area growth is still positive. However, premature senescence has occurred as a result of LAI 'kill' to remobilise nitrogen meet the demand for grain formation. This trend was also noted in the observations of LAI.

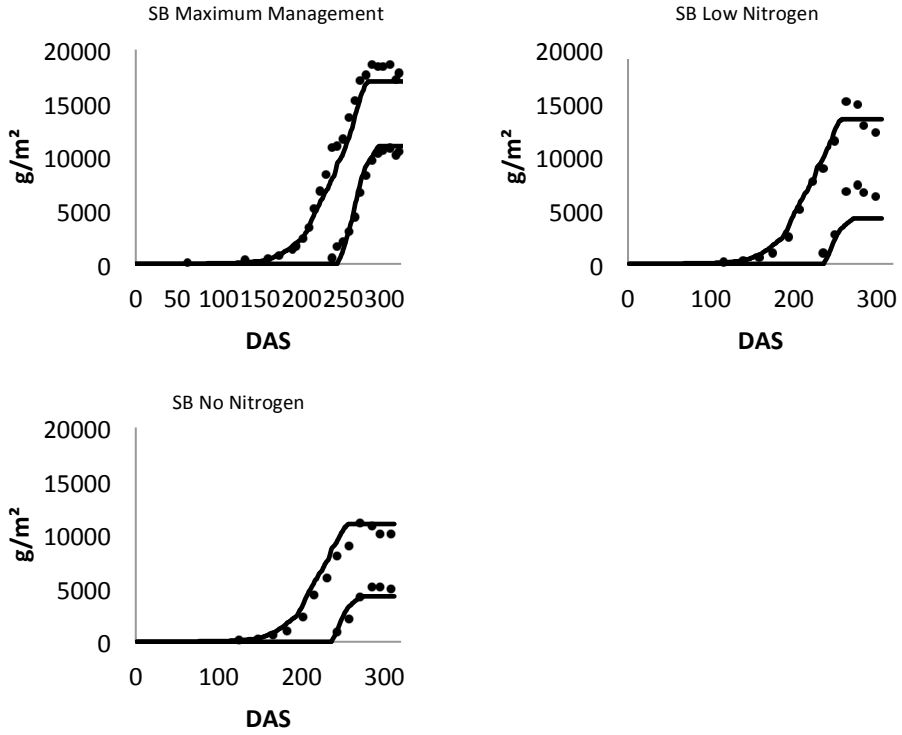


Figure 4.3 Time series of simulated (-) and observed (x) total and grain biomass (g/m^2). Grain biomass values are in the bottom right of all graphs. Weighted Mean Absolute Percentage Error (wMAPE) of 8.8% and 9.0% for total and grain biomass, respectively.

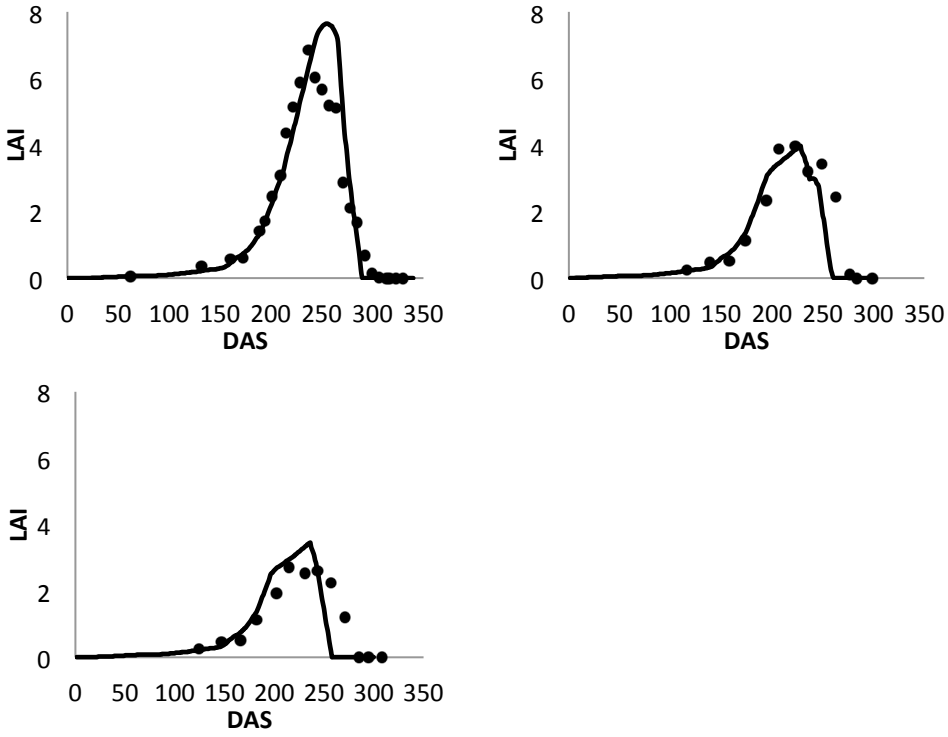


Figure 4.4 Time series of simulated (-) and observed (x) LAI. Weighted Mean Absolute Percentage Error (wMAPE) of 24%.

4.3.1.2 Cultivar Parameterisation

The fits achieved for individual cultivars were similar to those for Sirius (3.3.1). The average wMAPE for individual cultivars ranged from 22 (CF9107) to 39% (Quebon). Similarly to the complex model, the greatest error was attributed to LAI (Figure 4.5).

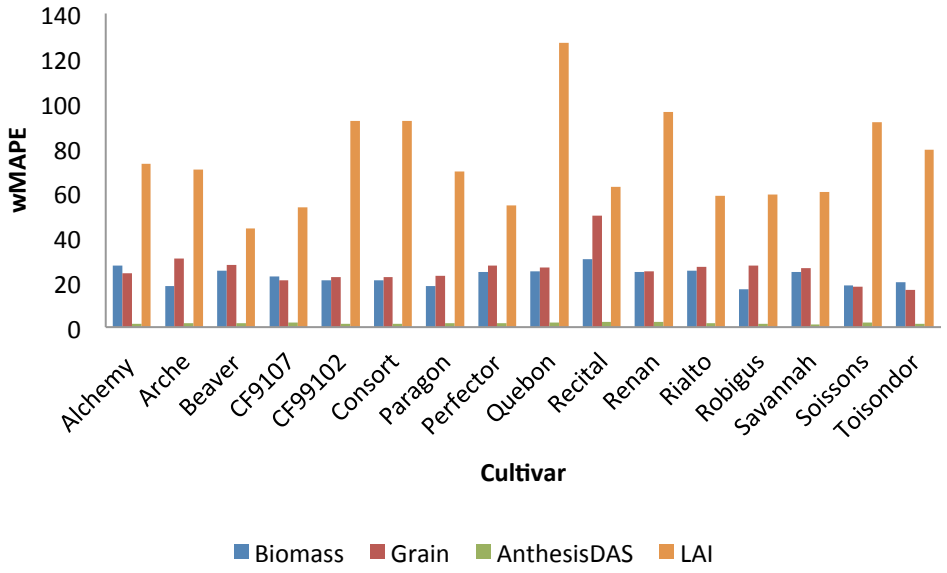


Figure 4.5 Weighted Mean Absolute Percentage Error (wMAPE) of biomass, grain yield, anthesisDAS and LAI of the best fitting parameterisation for each cultivar. Cultivars graphed in alphabetical order.

Parameter estimates for the intermediate model were more variable compared to the complex model (Table 4.2). As with the complex model, the vernalisation parameter of the intermediate model (P1V) had the greatest variability associated with its estimation (CV = 35%). The intermediate model also demonstrated a large number of significant inter-correlations between parameters *(data not shown)* and demonstrated similar sensitivity to starting points in the parameter space *(data not shown).*

Table 4.2 Average estimated parameter values for 16 cultivars. The estimated and coefficient of variation (CV) values represent the average for all 16 cultivars.

Parameter	Estimate	CV (%)
K_e	0.54	9
LAI_μ	1480	11
LAI_σ	345	26
LAI_0	4742	25
P1D	64	4
P1V	21	35
RUE	1.84	15
TTANTH	1138	3
TTANBGF	125	25
TTSOWEM	168	4
TTFLIN	471	7
TTBGEG	478	10

Overall, a more accurate simulation of cultivar growth and development was achieved for individual cultivars using the complex model (Table 4.3), with overall wMAPE values of 25% and 30% for the complex and intermediate models, respectively. The introduction of a simpler LAI sub-model resulted in a loss of accuracy in simulation of the canopy, with an increase in error of 45%. Relatively similar accuracy was achieved for the other modelled observations, with a small increase in the accuracy of predictions for biomass and anthesis date using the intermediate model, although grain yield predictions were slightly improved using the complex model (Table 4.3).

Table 4.3 Average Weighted Mean Absolute Percentage Error (wMAPE) achieved for 16 cultivars for model outputs using the intermediate and complex models

Model	Biomass	Grain	Anthesis	LAI
Intermediate	23	26	1.8	74
Complex	27	21	2.0	51

4.3.2 Farm Scale

The intermediate model was also applied to yield prediction at the farm level, using the dataset described in 2.9.1. As there was a lack of data regarding sowing and harvest dates and quantity and timing of fertiliser applications was not recorded, various assumptions had to be made, including that; (i) the winter wheat crop was sown on 1st October and harvested on 1st August, (ii) fertiliser expenditure was used as a proxy for application, as described in 5.5.4, and (iii) the fertiliser applications were split into three applications, as is commonly performed to coincide with important growth periods, with 25% applied in April and May and the remaining 50% applied in March (HGCA, 2009). Although daily temperatures (°C) were available, the other meteorological observations were only available on a monthly basis, and so it was assumed that radiation and rainfall were spread evenly throughout the month.

The model was particularly unable to simulate the range of yields of a number of farms (characterised by the segregated cluster in Figure 4.6), which were observed to have yields of 3 – 11.8 t ha^{-1}, but were predicted to only yield 2.5 – 4 t ha^{-1} (wMAPE = 18%). Analysis of the farms, indicated that this is potentially the result of higher than average rainfall and lower than average maximum and minimum temperatures associated with these farms, when compared to both the overall average of all farms and the average of all farms outside this cluster.

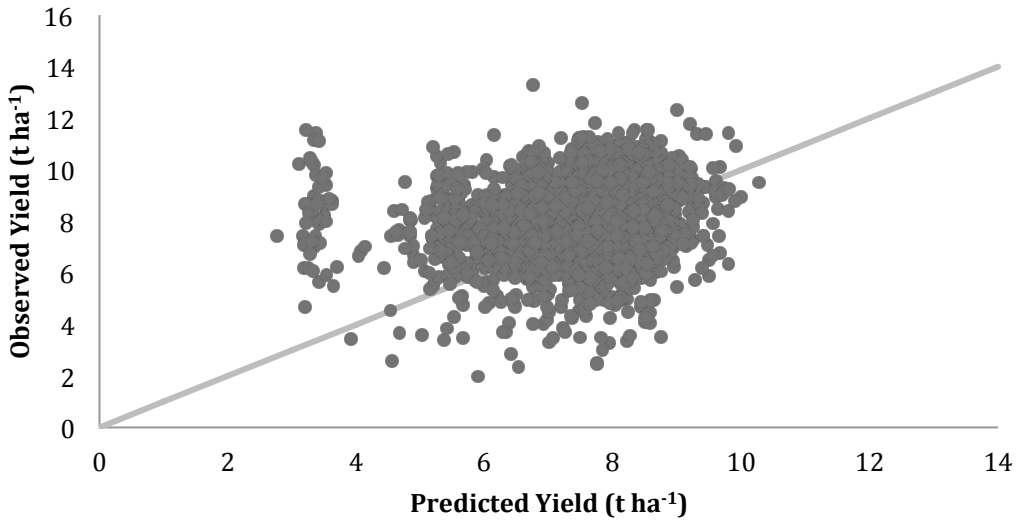


Figure 4.6 Application of the model of intermediate complexity to farm level yields following parameterisation. Weighted Mean Absolute Error (wMAE) = 1.48 t/ha, Weighted Mean Absolute Percentage Error (wMAPE) = 18%.

4.4 Model Reduction

Given the presence of a large number of significant parameter correlations and the parameter susceptibility to starting values, a model reduction analysis was performed in an identical manner to the complex model (Chapter 2.10), in order to identify model variables and parameters describing differences in phenology that are redundant in the context of the intermediate model.

4.4.1 Model Variables

A total of 72 variables were included in the screening analysis (Figure 4.7). Notable in this analysis is the large number of variables that only have a small detrimental effect on model SS_{res}, and conversely, the small number of variables that have a relatively large impact on SS_{res} ($0.9<SS_{res}$ ratio>1.5). In the analysis of the complex model, a large number of the variables produced a large impact on the SS_{res}.

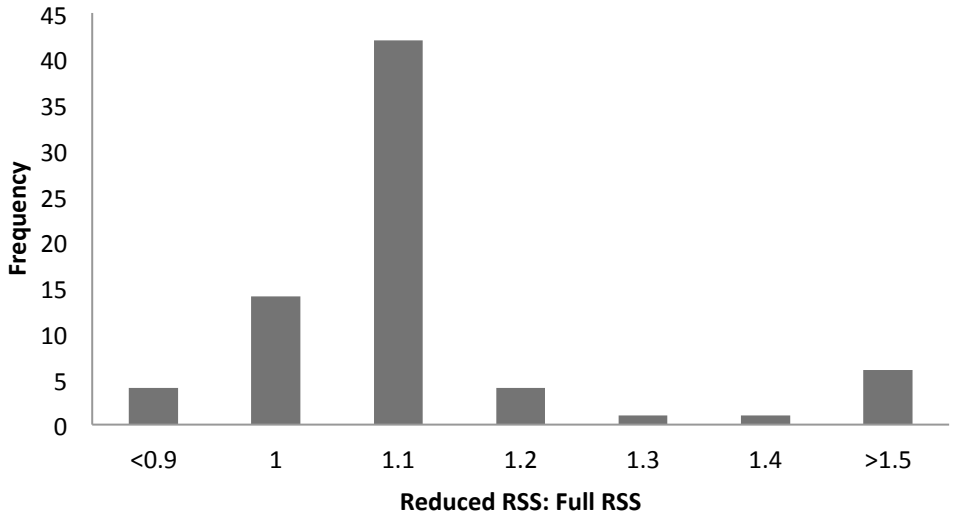


Figure 4.7 Frequency of the ratio of the reduced model SS_{res} to the full model SS_{res} for the 72 variables considered in the screening analysis

Analysis of the SS_{res} ratio identified 60 variables that produced a reduction in the ratio, or a small detrimental increase (<10%). Following mechanistic consideration of these variables, 10 were considered in the multi-factorial analysis. Assessment of the replacement probabilities for the candidate variables during the analysis was performed to check that relative stability had been achieved (Figure 4.8). The results are summarised in Table 4.4.

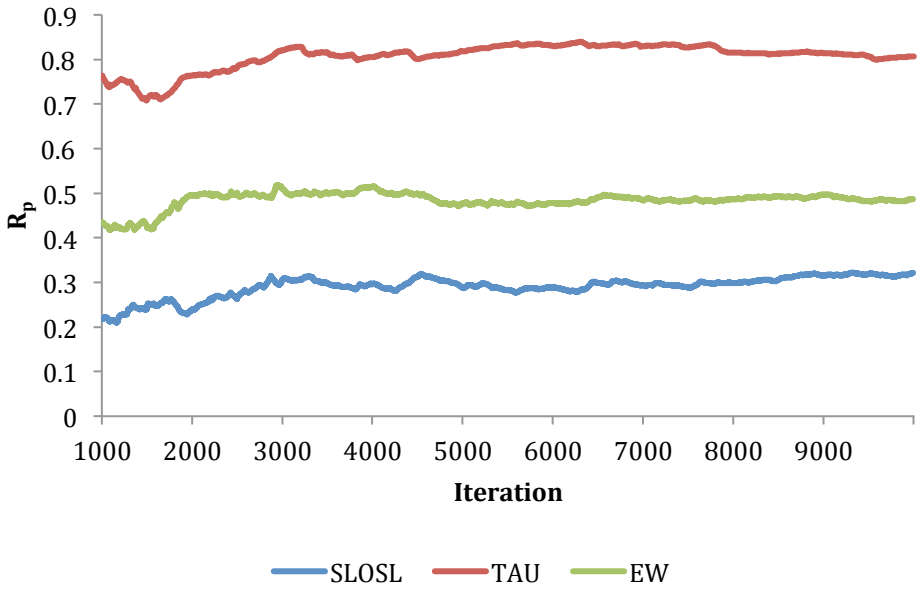


Figure 4.8 Replacement probability (R_p) evolution for selected candidate variables during the multi-factorial analysis.

Table 4.4 Candidate variables considered in the multi-factorial analysis.

Model Variable	Function	Min.	Max.	Replacement Constant		Replacement Probability
Nitrogen uptake						
LEAFDEMAND	Daily leaf area nitrogen demand calculation from leaf area expansion and leaf nitrogen requirements	0.00	8.80	7.19		0.03
Nitrogen mineralisation						
Fm	Factor representing the influence of soil moisture on nitrogen mineralisation	0.74	2.08	1.67		0.51
TMEAN_7	7-day moving average air temperature, used to calculate the effect of temperature on nitrogen mineralisation	0.24	22.1	5.07		0.50
Soil surface evaporation						
ALPHA	Factor representing the effect of canopy shading on soil surface evaporation	1.00	1.35	1.24		0.58
PTSOIL	Intermediate variable used in the calculation of soil surface evaporation	0	6.08	1.43		0.50
SLOSL	Intermediate variable used in the calculation of soil surface evaporation	0.00	39391	16.07		0.11
Evaporation						
EW	Intermediate variable used in the calculation of vapour pressure deficit, used in the calculation of evaporation	4.6	26.6	14.45		0.52
HSLOP_TMEAN	Intermediate variable used in calculation of evaporation	0.34	1.58	0.93		0.53
Vernalisation						
V_DAYS	Daily increment in number of vernalising days accumulated, used to calculate progress to full vernalisation	0.00	1.00	0.68		0.39

Model Variable	Function	Min.	Max.	Replacement Constant	Replacement Probability
S_VERN	Switch to remove the influence of vernalisation on crop development	-	-	0	0.33

Although the nitrogen uptake variable LEAFDEMAND, describing the requirements for non-limited leaf area expansion, was included in the multi-factorial analysis, it had a very low replacement probability (R_p=0.03), indicating that model predictive ability was improved when this variable was not replaced. Similarly to the complex model, variables describing the influence of soil moisture and temperature on nitrogen mineralisation were identified as redundant, as were a number of evaporation variables. One variable used to calculate soil surface evaporation (SLOSL) was indicated to improve model performance (R_p=0.11). In the analysis of this intermediate model however, switching off the simulation of vernalisation effects (S_VERN) was not demonstrated to be redundant, indicating that the inclusion of this process improved the models predictive ability. The vernalisation variable V_DAYS was also judged not to be redundant (R_p=0.39).

4.4.2 Cultivar Parameters

As in the complex model, a number of parameters designed to describe differences in cultivar growth and development were identified as potentially redundant.

Thermal time constants describing emergence (TTSOWEM) and the time between anthesis and the beginning of grain filling (TTANBGF) were excluded from the multi-factorial analysis (SS_{res} ratio>1.1). The multi-factorial analysis identified redundancies in six parameters (Table 4.5), including those describing vernalisation (P1V), thermal time durations (TTFLIN, TTBGEG) and canopy characteristics (LAI_μ, LAI_0 and K_e). Low replacement probabilities associated with the parameters

describing daylength (P1D), thermal time to anthesis (TTANTH) and canopy duration (LAI_{σ}) indicated that these were important in describing differences between cultivar growth and development. RUE was borderline redundant (R_p=0.43).

The analysis indicated that model predictive ability could be maintained by only considering six of the parameters as cultivar-specific and replacing the remaining six with constants (i.e. that do not differ between cultivars). The resulting model would describe differences in cultivar growth and development as a function of parameters describing photoperiod sensitivity, thermal time to emergence and anthesis from sowing, as well as thermal time between anthesis and grainfill start, canopy duration and radiation use efficiency.

Table 4.5 Parameters used to describe cultivar differences (included as variables) during multi-factorial analysis

Model Variable	Function	Min.	Max.	Replacement Constant	Replacement Probability
Daylength					
P1D	Photoperiod sensitivity	48	65	62	0.32
Vernalisation					
P1V	Vernalisation requirement	11	22	30	0.53
Thermal Time Constants					
TTANTH	Thermal time duration of the period from emergence to anthesis	1070	1300	1229	0.24
TTFLIN	Thermal time duration from emergence to floral initiation	116	190	500	0.56
TTBGEG	Thermal time duration of the period from beginning of grainfill to the end of grainfill	400	650	522	0.55
Canopy					
LAI_{μ}	Canopy timing	912	2402	1160	0.62
LAI_{σ}	Canopy duration	228	471	256	0.36
LAI_0	Canopy size	4012	9200	2984	0.77
Dry Matter					
RUE	Radiation use efficiency	1.20	2.41	1.2	0.43
K_e	Extinction coefficient of the crop canopy	0.45	0.62	0.45	0.55

4.5 Conclusion

The intermediate model was able to simulate wheat growth and development under nitrogen limiting conditions considerably better than under water limiting conditions,

indicating that this model of intermediate complexity is more suited to application in temperate climates, which are less likely to suffer significant drought effects. This deficiency is linked to the simplification of the soil profile and associated water dynamics. In the intermediate model, the soil is considered as one layer, rather than the multi-layer, tipping bucket approach favoured by complex models, such as Sirius. A number of simplifications were made from relationships contained within this more complex model,

Parameterisation of the intermediate model for the 16 cultivars demonstrated that the explicit simulation of individual leaves, as in the complex model, is not necessary to achieve similar accuracy in predicting biomass, grain yield and anthesis date. Although there was an associated reduction in the accuracy of LAI simulation.

The main differences between the complex and intermediate models were the simplification of descriptions for; (i) temperature effects, (ii) vernalisation and daylength, and (iii) the soil profile. Both the complex and intermediate models demonstrated potential for redundancy, both when model variables and cultivar-specific parameters were considered.

Of the 72 model variables considered, only six were identified as potentially redundant. These included variables describing evaporation and soil nitrogen mineralisation. The vernalisation variable and switch included in the multi-factorial analysis were not assessed as redundant. However, analysis of the cultivar-specific parameters identified vernalisation requirement as potentially redundant. Therefore, although use of a generic vernalisation requirement did not affect model predictive power, the analysis indicated that the removal of the simulation of vernalisation effects completely was detrimental to model predictions.

In addition to the parameter describing vernalisation requirement, a further five parameters were identified as potentially redundant, suggesting that cultivar differences could be explained by this model using three thermal time parameters, and parameters describing photoperiod sensitivity, canopy duration and radiation use efficiency.

The intermediate model was also applied at the farm level, although this required a number of assumptions to be made due to a lack of observations that are traditionally provided to mechanistic crop models (e.g. daily meteorological observations). The effect of these assumptions, i.e. regarding sowing, harvest and fertiliser application dates, on model predictions should be quantified. At this level, the model was unable to simulate the full range of observed yields of a particular subset of farms, which was linked to these farms experiencing rainfall and temperatures that were notably different from the average.

5 A New Empirical and a New Mechanistic Model: Farm-Scale

Previous chapters (3 & 4) have focused on the application, and reduction of, mechanistic models at the field-scale, using datasets obtained from field trials. Rather than attempting to apply (and adapt) existing models developed for use at the field-scale, this chapter focuses on developing new models for predicting yield at the farm-scale for the data - nationally collected climate and farm management information - that is available. In this chapter, both empirical and mechanistic modelling approaches are considered. As each type has different data requirements and sensitivities (Watson et al., 2015; Estes et al., 2013b), and have been demonstrated to produce differing yield predictions under projected climates (Morin & Thuiller, 2009; Estes et al., 2013b; Giardin et al., 2008), it has been suggested that application of both model types will allow a complete picture of the crop-climate response (Estes et al., 2013a; Estes et al., 2013b; Watson et al., 2015; Morin & Thuiller, 2009; Giardin & Tardif, 2008).

The formulation of a new mechanistic model for use at the farm-scale, rather than application of an existing field-scale model, allows careful consideration of the processes and level of detail to include, given the broader scale of interest and the data available at this scale.

The following work was written up in paper format under the title 'predicting on farm wheat yields; development and comparison of a empirical and a

mechanistic modelling approach'. It is included below in that format. Additional discussion is included in Chapter 6.

5.1 Introduction

Wheat is one of the most important food crops in the world, contributing nearly 30% of global cereal production (FAO, 2013). As a result, there have been many attempts to predict wheat yields using different modelling approaches. These range from relatively simple, empirical models, derived from large observational datasets (e.g. Lobell and Burke, 2010) to detailed, mechanistic models, which describe large numbers of interacting biophysical process (e.g.Vanuytrecht et al., 2014).

Mechanistic models are widely used in modern cereal modelling research (Mirschel et al., 2014). The simulated crop's growth is usually driven by radiation interception and conversion into leaf area and biomass, with the development typically described using temperature-derived thermal time. This growth is often restricted by nutrient (primarily nitrogen) and water uptake, which is affected by their availability in the soil profile as a function of root growth and development and soil characteristics (e.g. Jamieson et al., 1998a). These complex models usually require a large number of parameters describing cultivar, management and soil characteristics. Therefore, datasets typically require detailed phenological and growth observations over time, as well as soil texture, water availability and inorganic and organic nitrogen quantities. This can make them difficult to calibrate and limited calibration can result in poor model performance (Palosuo et al., 2011). Empirical models are derived from large, often historical datasets primarily containing yield and climate data to produce relatively simple regression equations describing the relationships between these variables (Lobell & Burke, 2010). Therefore, simpler empirical models can be

advantageous in their requirement for less detailed (albeit numerous) data, especially at broader scales, when the detailed field and/or laboratory-derived parameters of mechanistic models are difficult to define (Lobell and Burke, 2010; Mirschel et al., 2014). For example, Landau et al. (1998) developed a simple regression model to predict British wheat yields that required only monthly climate data as inputs. However, as statistical models explain, rather than describe the relationships between yield and growing season climate, their application is restricted to the climate in which they were developed.

Primarily, cereal modelling has focused on the application of models developed using research trial data to field (e.g. Jamieson et al., 1998b) and large scale yield forecasting (e.g. Challinor et al., 2004). There has been much less effort directed towards the prediction of yields using farm observations or the investigation of controlling factors for yield in the farm situation (Mirschel et al., 2014). The availability of suitable observational data is an obvious reason for this omission but it may also reflect the desirability of controlled conditions for physiologically orientated research directed towards increasing yield potential. An alternative approach is to utilise farm data collected for the development of official statistics. A few authors have used this approach to test and parameterise mechanistic crop models (e.g. Klein et al., 2012; Lehmann and Finger, 2014), however examples of this approach for model development are lacking (Mirschel et al., 2014).

Our aim is to investigate the prediction of farm wheat yields using nationally collected meteorological and farm management information. We present the development of two winter wheat *(Triticum aestivum)* yield prediction models parameterised with farm statistics, using an empirical and a mechanistic approach, respectively.

Although the models developed in this study are restricted in their application to England and Wales, where the data were collected, the approach is widely applicable where suitable data is available.

5.2 Data Sources

5.2.1 Farm Business Survey

The England and Wales Farm Business Survey (FBS) collects financial and physical data for all types of farms across England and Wales to underpin both national policy requirements and contribute to the European Farm Accountancy Data Network (DEFRA, 2013a). Data collected include farm, cropping and forage areas, stocking, production, sales and expenditures. This information is collected from farm management records and accounts together with face-to-face interviews with farmers and is provided for development and analysis of policy, business advice, benchmarking and research.

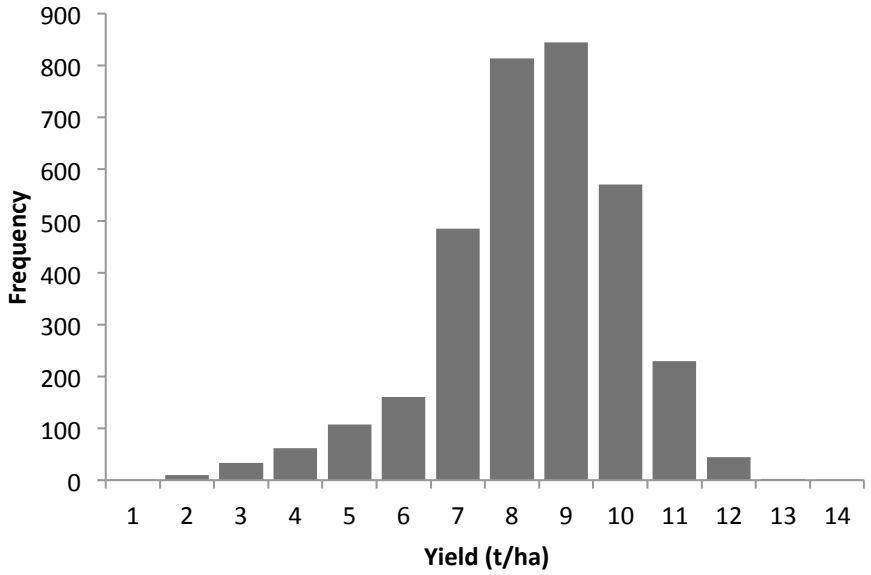


Figure 5.1 Distribution of the observed yields (n = 3367) over the period 2005-2010. The mean yield was 7.88 t ha^{-1}, with a standard deviation of 1.7t ha^{-1}.

The dataset used for this project included 3,367 yield observations from 700 farms over the period 2005-2010 (Figure 5.1). The farm location is only identified within the data to the nearest 25x25km within the UK's national grid reference system to ensure farm anonymity (Figure 5.2). Data were obtained from the FBS database for; farm and wheat cropped area, wheat yield, output value of the wheat crop, variable (seed, fertiliser, crop production and other costs) and fixed (labour, machinery, land and contract) costs, as well as farm / farmer characteristic data (farmer age, farmer education level, organic status of farm and organic enterprises on farm, plus an estimated livestock waste, i.e. manure/slurry, applied to the wheat crop). Monetary output value and input cost data were deflated to 2010 levels to remove inflationary / deflationary effects on agricultural input and output prices (DEFRA, 2015). The dataset was split into a development sample (75%, n=2525) used for parameterisation and a test sample (25%, n=842), used to conduct an independent assessment of the models. Data splitting is commonly used during model development (e.g. Guillaume et al., 2011; Kumar et al., 2015; Landau et al., 2000) and although there is no consensus on the optimal split, which is a function of the project dataset size and detail as well as the model being developed, it has been demonstrated that assigning more of the dataset to the development sample reduces model uncertainty (Sun and Bertrand-Krajewski, 2012).



Figure 5.2 Locations of surveyed farms (n=3367) used for this study in England and Wales. Symbols indicate farms with yield observations included in the development (o) and test (x) samples, as explained in the text. Multiple farms can be present at one location due to the use of a 25x25km grid.

5.2.2 Meteorological Data

Monthly mean values of maximum and minimum temperatures (°C), sunshine hours (hours), and rainfall (mm) were obtained on a 5x5km national grid basis from the UK Met Office for October 2005 to July 2010 (MetOffice, 2014). The data are derived from an observational network using an interpolation process (Perry and Hollis, 2004). Monthly solar radiation (MJ ha^{-1}) was estimated from the monthly sunshine hours using the FAO method (Allen et al., 1998). Values for the 25x25km grid (farm locations) were estimated as an average of these 5x5km data.

5.3 Method

The predictive performance of the models was measured using the adjusted coefficient of determination (r^2_{adj}), mean absolute error (MAE) and mean absolute percentage error (MAPE)(Section 2).

$$r^2{}_{adj} = 1 - \frac{(\sum(O_i - P_i)^2)/(n-1)}{(\sum(O_i - \bar{O})^2)/(n-p-1)}$$

Equation 5.1

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|O_i - P_i|$$

Equation 5.2

$$MAPE = \frac{100}{n}\sum_{i=1}^{n}\left|\frac{O_i - P_i}{O_i}\right|$$

Equation 5.3

Where n is the number of observations, O_i is the *i*th observation, $\bar{O}$ is the mean of the observed values, W_i is the weight associated with the *i*th observation and P_i is the *i*th predicted value.

Additionally for the empirical model, the explained yield variance was decomposed to assess the relative importance of each fitted variable.

As no sowing or harvest date was recorded, it was assumed that the winter wheat crop was sown on 1st October and harvested on 1st August, (i.e. climate data for August and September was excluded from the models).

5.4 Empirical Model (Simple-EMP)

5.4.1 Model Development

Previous empirical models have focused on climatic factors as driving variables (Landau et al., 1998). Here, a multiple regression model (Simple-EMP) was developed using a mixture of climate and farm management variables. The potential explanatory variables considered are summarised in Table 5.1, and were selected based on consultation with an experienced FBS researcher (*P.Wilson, pers. comm.).* The statistical software Minitab® was used to select variables by stepwise regression for inclusion in the model when their variance ratios were significant at the 5% level. In addition to these variables, interaction terms were considered for crop protection, seed, fertiliser and manure expenditures to explore the potential interaction between variable inputs (e.g. increased seed input costs may lead to lower weed burden and hence lower crop protection costs).

Two variables describing the farm size were included, together with farmer age and education level, the farm's organic status, and the presence of organic enterprise(s). A number of expenditures, ranging from costs associated with purchasing seeds, fertilising and protecting the crop to expenditure on contractors, labour and land were included. A range of variable costs incurred by the farmer were represented in the data by the variable 'other'. A further source of fertiliser was also considered in the form of livestock manures, as the dataset contained farms that had both wheat and livestock enterprises. These farms may be applying on-farm produced manures, with potential effects on the yields recorded not captured by their fertiliser expenditure. In order to estimate this effect, livestock numbers for individual farms were determined from livestock unit values recorded in the FBS. It was assumed that all livestock manure produced during the housing period was applied, up to a maximum of 250 kg ha^{-1} (inclusive of any fertiliser applied), to comply with policy (DEFRA, 2010).

Quantities of manure were determined using average published values for livestock waste produced during this housing period (DEFRA, 2010).

Finally, it was hypothesised that a farm's use of fertiliser may be related to the relative cost of fertiliser and the value of grain. To include this as a potential explanatory variable, a wheat-fertiliser price ratio (WF_{ratio}) was calculated (Equation 5.4).

$$\boldsymbol{WF_{ratio} = \frac{DWP}{DP_F}} \qquad \textbf{(Equation 5.4)}$$

Where DWP is the Deflated Wheat Price, calculated by dividing the deflated value of wheat yield (Y_{value}, £) by the total wheat production (P_{total}, t). DP_F is the deflated index of fertiliser prices.

All continuous explanatory variables were centred around their means, to aid interpretation of the fitted coefficients in a fashion similar to Landau et al. (2000). Categorical explanatory variables were included in the regression as indicator variables. Expenditure and rainfall variables were log(+1) transformed to reduce skew as a result of zero values. Both variables are frequently transformed in this manner when incorporated into regression models to meet the assumptions of normality required (e.g. Landau et al., 1998; Landau et al., 2000).

Table 5.1 Explanatory variables considered in the development of the empirical model, Simple-EMP.

Variable	Description
Climate	
Maximum temperature	Monthly mean maximum temperature (°C, October – July)
Minimum temperature	Monthly mean minimum temperature (°C, October – July)
Rainfall	Monthly mean rainfall (mm, October – July)
Sunshine Hours	Monthly mean sunshine hours (hours, October – July)
Size	
Wheat area	Current cropped wheat area (ha)
Farm area	Total utilisable agricultural area (ha). Includes cropped, set-aside and grassed areas.
Expenditure	
Seeds	Seed expenditure (£/ha)
Fertiliser	Fertiliser expenditure (£/ha)
Crop Protection	Crop protection expenditure (£/ha). Includes insecticides, herbicides, fungicides and growth regulators.
Other	Other variable expenditure (£/ha). Includes feedstuffs, fodder, veterinary care, other crop costs (e.g. wire and twine) and heating fuel.
Contractor	Contract work expenditure (£/ha)
Machinery	Total machinery costs (£/ha). Includes rental costs, repairs and fuel.
Land	Total land expenses (£/ha). Includes tenant repairs, upkeep of land, rental costs.
Labour	Expenditure on casual labour (£/ha). Includes paid and unpaid labour of farmer, spouse, manager and other employees.
WF_{ratio}[1]	Wheat-Fertiliser price ratio
Other	
Organic[2]	Type of organic enterprises present on farm: categorised as (1) no organic enterprises, (2) all enterprises organic, (3) dairy, (4) beef, (5) sheep, (6) poultry, (7) pigs, (8) potatoes, (9) wheat, (10) field beans, (11) field scale vegetables, (12) protected cropping, (13) other.
Age	Age of farmer (years)
Education[2]	Education level of farmer: categorised as (1) basic – no further/higher education, or (2) higher – college, diploma or degree level education.
Manure[1]	Estimated livestock waste applied to cropped wheat area (t/ha)

[1]estimated as described in 5.4.1 [2]recorded categorically, therefore included in the model as indicator variables

5.5 Mechanistic Model (Simple-MECH)

The approach to the processes and driving variables considered in the mechanistic model (Simple-MECH) are described below, with adjustable model parameters summarised in Table 5.2. Different model designs were considered building on a

base model with a monthly time-step, containing the driving temperature and radiation descriptions. Each effect was considered individually, before progressively more complex model designs, describing more processes and requiring parameters, were considered using multiple effects (Table 5.4). The maximal model described wheat growth as driven by radiation and temperature, with the potential for water-limited growth (5.5.2), loss of biomass under high rainfall (5.5.3) and enhanced canopy size with increased fertiliser and crop protection expenditure (5.5.4-5.5.6).

Each model design was parameterised using the Metropolis-Hastings algorithm in OpenModel with the development dataset (Van Oijen et al., 2005). The OpenModel software is designed to allow the parameterisation and analysis of mathematical models, with the facility to read the spatial meteorological data used in this study (Tarsitano et al., 2011).

5.5.1 Temperature and Solar Radiation

The model relates biomass growth to estimated solar radiation and temperature using the classical model of light interception and conversion (Monteith, 1969):

$$\frac{dB}{dt} = Growth = RUE \times Rad\left(1 - \exp\left(-kL\right)\right) \qquad \textbf{Equation 5.5}$$

Where B is the crop dry weight biomass (t ha^{-1}), growth is the monthly increase in biomass (t ha^{-1} $month^{-1}$), RUE is radiation use efficiency (t DM MJ^{-1} intercepted light), Rad is the solar radiation (MJ m^{-2} $month^{-1}$), k is the canopy extinction coefficient and L is the canopy leaf area index. In this study, the canopy extinction coefficient was fixed at 0.5.

The canopy leaf area index, L, is estimated using a model which relates the rate of change of L to the thermal time experienced by the crop (Gillett et al., 1999):

$$L = \frac{LAI_{int}}{LAI\sigma\sqrt{2\pi}} e - 0.5(\frac{T_t - LAI\mu}{LAI\sigma})^2$$ **Equation 5.6**

Where T_t is the accumulated thermal time from sowing, LAI_{int}, LAI_{σ}, and LAI_{μ} are parameters which describe the canopy size, duration and timing, respectively. Gillett et al (1999) present estimated values of these parameters for cv. *Mercia*. During parameterisation, potential estimates for LAI_{int} were restricted to the range of those estimated for this cultivar.

Yield, Y, is calculated from crop biomass using a harvest index parameter HI_0 (Equation 5.7), which was fixed at 0.5.

$$Y = HI_0 \times B$$ **Equation 5.7**

5.5.2 Drought

Drought is not a major constraint to UK wheat production, although approximately 10% of wheat yield is lost annually as a result of insufficient soil moisture. This deficiency of water during critical stages of yield formation prevents attainment of potential yields (Ober et al., 2013).

The potential influence of drought is included through calculation of a water use requirement for the crop. The soil (at all locations) is assumed to have a store of water, SW (mm of water). The water use required to support the growth predicted by

light interception, WU, is calculated using the concept of transpiration equivalent TE (kg ha^{-1} mm^{-1}) (Azam-Ali et al., 1994):

$$WU = \frac{growth}{TE}$$ **Equation 5.8**

This water use is met through rainfall, R, and if this is not sufficient to fully meet the required water use of the crop, the difference is met by a reduction in the stored soil water:

$$\frac{dSW}{dt} = R - WU$$ **Equation 5.9**

This is subject to two constraints; (i) that SW cannot exceed the maximum storage capacity of the soil (SW_{max},) and (ii) that SW≥0, so when the stored water is reduced to zero, crop growth is restricted.

5.5.3 High Rainfall

High rainfall can be detrimental to yield through increased likelihood of disease and/or lodging and in their empirical model Landau et al. (2000) found significant negative effects of rainfall on potential yield. This possibility is considered here by calculating a monthly loss of biomass, ΔB, assuming that damage can occur if biomass exceeds a threshold B_d and monthly rainfall exceeds R_d (Equation 5.10), i.e. that large canopies are susceptible to damage from high rainfall.

$$\Delta B = D \times B \qquad \boldsymbol{R > R_d; B > B_d}$$ **Equation 5.10**

Where D represents the proportion of the crop biomass which is lost due to rainfall damage.

5.5.4 Fertiliser

Fertiliser applications provide key nutrients, such as nitrogen, at important stages of crop development. The effect of applied fertiliser is assumed to operate through canopy size. Gillett et al. (1999) considered this in their canopy model, empirically relating the parameter LAI_{int} to nitrogen available to the crop, $N_{tra,}$ whether by direct application or as soil nitrogen:

$$LAI_{int} = a_1 + a_2 N_{tra}$$ **Equation 5.11**

Where a_1 and a_2 are empirical parameters, which Gillett et al. (1999) estimated by fitting the model to a series of experimental studies in which detailed sequential growth analysis observations were made for cv. Mercia.

Total applied nitrogen is not known from the survey data; instead the cost of fertiliser, C_F (£ ha^{-1} deflated for inflation) was used as a proxy for nitrogen application. Direct application of the above equation was not considered appropriate as it implies an unbounded increase in maximum canopy size (through LAI_{int}) as nitrogen application increases and this is unrealistic. Therefore an alternative description was used to relate LAI_{int} and C_F:

$$LAI_{int} = LAI_0 \left(1 + A_{fert}\left(1 - exp\left(-\frac{C_F}{K_{fert}}\right)\right)\right)$$ **Equation 5.12**

Where LAI_0 represents the maximum canopy size in the absence of fertiliser, A_{fert} represents the proportion of LAI_0 attributable to fertiliser application and K_{fert} is a shape parameter.

5.5.5 Manure

Estimated applied manure (A_M) was related to LAI_{int} using the previously described relationship (Equation 5.12). When both fertiliser and manures are considered, they are assumed to have an additive effect:

$$LAI_{int} = LAI_0\left(1 + A_{fert}\left(1 - exp\left(-\frac{C_F + A_M}{K_{fert}}\right)\right)\right) \quad \textbf{Equation 5.13}$$

5.5.6 Crop Protection

In typical farming practice, a number of agro-chemicals are applied to protect the crop from pests and diseases. As well as fungicides, insecticides and herbicides, growth regulators are also applied (DEFRA, 2013b). The relevant recorded information is the cost of sprays applied (C_s). The model assumes this to have a role in protecting the canopy using a similar relationship to that described above for fertiliser (Equation 5.12). When both spray and fertiliser are considered together in the model, they are assumed to interact:

$$LAI_{int} = LAI_0\left(1 + A_{fert}\left(1 - exp\left(-\frac{C_F}{k_{fert}}\right)\right)\right)\left(1 + A_{spray}\left(1 - exp\left(-\frac{C_S}{k_{spray}}\right)\right)\right)$$

Equation 5.14

Table 5.2 Adjustable model parameters considered during Simple-MECH model selection process.

Parameter	Description	Unit	Initial Value	Bounds
Temperature and Radiation				
RUE	Radiation Use Efficiency	t MJ^{-1}	1.5	n/a
LAI_0	Canopy Size	°Cdays	6700	2760 - 10396
LAI_μ	Canopy Timing	°Cdays	1631	n/a
LAI_σ	Canopy Duration	°Cdays	381	n/a
Drought				
TE	Transpiration Equivalent	kg ha^{-1} mm^{-1}	20	n/a
SW_{max}	Maximum storage capacity of the soil	mm	150	n/a
High Rainfall				
R_d	Rainfall threshold	mm	100	1-1000
B_d	Biomass threshold	t ha^{-1}	10	n/a
B_l	Proportion of biomass lost	-	0.5	0.05 – 1
Fertiliser				
A_{fert}	Proportion of canopy size attributable to fertiliser and/or manure application	-	0.5	0 - 1
K_{fert}	Shape parameter	-	50	n/a
Crop Protection				
A_{spray}	Proportion of canopy size attributable to spray application	-	0.5	0 - 1
K_{spray}	Shape parameter	-	50	n/a

5.6 Results

5.6.1 Simple-EMP

The results from the regression analysis are summarised in (Table 5.3). The empirical yield-climate-management model, Simple-EMP, was able to explain 42% of the variation in observed farm yields in the development dataset and 41% in the independent test dataset (Figure 5.3). Although 23 variables were fitted, 10 of these each contributed less than 1% of the explained variation. 80% of the explained variation was accounted for by four fitted variables; (i) crop protection expenditure, (ii) minimum temperature in March, (iii) farm area and (iv) rainfall in January. Crop protection expenditure positively impacted on yield and was the most important variable, accounting for nearly 60% of the variation explained.

Table 5.3 Explanatory variables[1] included in the empirical model (Simple-EMP) developed using monthly meteorological and annual farm management data (r^2adj = 0.42, MAE = 1.03t ha^{-1}, MAPE= 15.1%). The standard error (s.e.) of each significant variable's coefficient and the percentage of sequential sum of squares accounted for by each variable (importance) were determined.

Predictor[2]	Coefficient	s.e.	Importance (%)
Constant	7.33	0.18	
Crop protection expenditure[3]	0.78	0.15	57.65
Min. temperature in March	-0.60	0.06	13.66
Farm area[3]	0.58	0.07	5.91
Rainfall in January[3]	-0.92	0.16	3.55
Max. temperature in May	-0.26	0.03	2.22
Other expenditure[3]	0.28	0.04	2.22
Rainfall in June[3]	-0.63	0.13	1.73
Machinery expenditure[3]	0.49	0.06	1.66
Spray-Fertiliser Interaction	0.35	0.05	1.46
Radiation in October	-1.07	0.15	1.24
No Organic	0.56	0.19	1.09
Manure [3]	-0.14	0.03	1.05
Land expenditure[3]	0.87	0.12	1.04
Organic Dairy	3.55	0.93	0.94
Contractor expenditure[3]	0.17	0.03	0.92
Max. temperature in July	0.33	0.04	0.83
Radiation in November	0.89	0.18	0.71
Organic Sheep	-2.01	0.75	0.42
Min. temperature in May	0.44	0.07	0.42
Spray-Manure Interaction	-0.20	0.08	0.39
Radiation in April	-0.13	0.05	0.36
WF_{ratio}[3]	-0.33	0.10	0.28
Max. temperature in April	-0.08	0.04	0.26

[1]centred around their mean [2]significant at $p<0.05$ level [3]log transformed.

Overall, management variables were more important predictors than climate, accounting for 74% of the variation explained. Positive effects on yield were estimated for crop protection, other, machinery, land and contractor expenditures. Manure application was estimated to reduce yields. Two interactions were included in the model, crop protection x fertiliser expenditure and crop protection expenditure x manure application, having a positive and negative impact on yields, respectively.

Fertiliser expenditure was not included in the final model as a single factor. However, there was a highly significant correlation between fertiliser and crop protection expenditure ($p<0.001$) and further investigation found that it was included in the model as a single factor if crop protection expenditure was not considered. This produced a model that accounted for almost as much variation in yield as that described above ($r^2_{adj}=0.40$).

The absence of organic enterprises or the presence of an organic dairy on a farm was estimated to have a positive impact on yield. However, the presence of organic sheep on the farm was estimated to reduce yields. A negative effect on yield was estimated for WF_{ratio}. Of the farm management variables considered, those with no effect on yield (and therefore not included in the statistical model) included wheat area, seed and labour expenditure, farmer age and education status and a number of organic enterprise types.

5.6.2 Simple-MECH Model

Of the model designs considered, the base model of temperature and radiation was unable to simulate the observed farm yields ($r^2_{adj}<0$). Addition of a drought or manure application description (Base+Drought, Base+Manure) did not improve the model's explanatory ability (Table 5.4). Consideration of a rain damage effect (Base+HighRain) during the simulation was only able to account for 1% of the variation in observed yields, however designs including effects of fertiliser and crop protection expenditure (Base+Fertiliser, Base+CP) improved the model's explanatory power considerably. When both effects were considered together, the resulting model (Base+Fertiliser+CP) accounted for 26% of the observed variation in yields. The explanatory power of the model was then further increased by including a rain

damage effect in the model design (Base+HighRain+Fertiliser+CP, r^2=0.27). Although many different combinations were considered, this model produced the best fit to the observed yield data and explained 25% off the observed variation when applied to the independent test dataset (Figure 5.3).

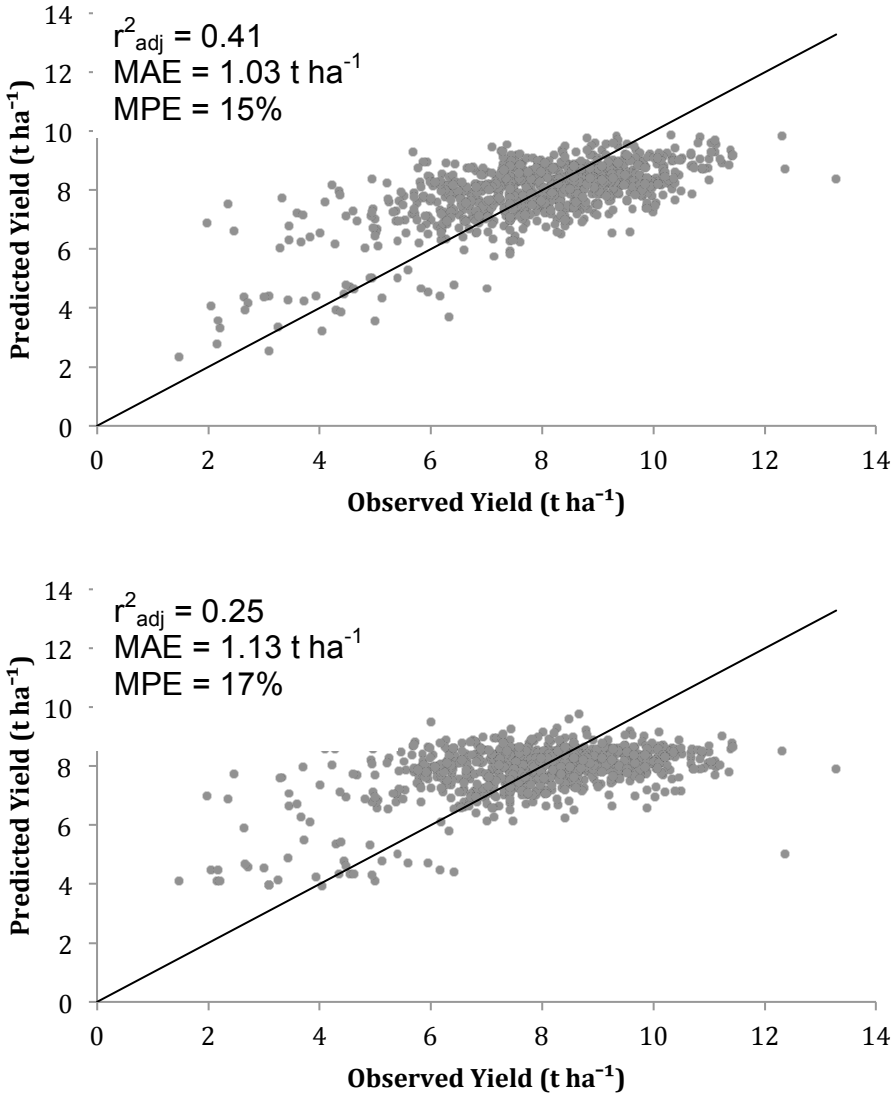


Figure 5.3 Yields predicted by the empirical (Simple-EMP) (a) and mechanistic (Simple-MECH) (b) models plotted against observed grain yields in the test sample (n=842). The 1:1 line is shown representing perfect agreement.

Table 5.4 Simple-MECH model designs considered during model development. The selected model with the greatest predictive power (r^2_{adj}=0.27) included a high rainfall (HighRain), fertiliser and crop protection (CP) effect on top of the Base model.

Effects Considered	Base	Base +Drought	Base +HighRain	Base +Fertiliser	Base +Manure	Base +CP	Base +Fertiliser +CP	Base +HighRain +Fertiliser +CP
Temperature & Radiation	x	x	x	x	x	x	x	x
Drought		x						
High Rainfall			x					x
Fertiliser				x			x	x
Crop Protection						x	x	x
Manure					x			
r^2_{adj}	-0.02	-0.02	0.01	0.18	-0.02	0.24	0.26	0.27
MAE	1.31	1.30	1.28	1.19	1.30	1.15	1.14	1.13
MAPE	21.1	21.0	20.8	18.1	21.0	17.3	16.9	16.8

5.7 Discussion

Both developed models were unable to replicate the full range of yields observed, indicating that there is some key source of yield variability that is not captured in either case. This bias is more pronounced for the mechanistic model (Figure 5.3). Although observed yields ranged between 1.00-13.3 t ha^{-1}, the simulated yields had narrower ranges of 2.12-10.7 t ha^{-1} and 3.59-9.86 t ha^{-1} for the empirical and mechanistic model, respectively.

It has been demonstrated previously that models can be insensitive to, or show considerable bias to, aggregation of soil and climatic data, and therefore individual model assessment is required (Hoffman et al., 2016). Climatic data generated by averaging (as here, from 5x5km to 25x25km) can result in a loss of spatial variability, and use of monthly values, a loss of temporal variability (Ewert et al., 2011). The effect of averaging of these model inputs was not considered here, but should be explored to assess whether this may have contributed to the bias noted. Although it was considered here during development of the statistical model, averaging soil information is not meaningful, due to the non-linear relations between soil variables (Hoffman et al., 2006).

5.7.1 Simple-EMP Model

Previous attempts to simulate wheat yields from large observational datasets in the UK using monthly climate-based regression models developed under optimal management have produced consistent results. Using development datasets, 32% of the variation in multiple site (Landau et al., 1998) and 35% of the variation in single site (Chmielewski and Potts, 1995) yield observations accounted for in the development datasets. Although no independent test of the empirical model of

Landau et al. (1998) was performed, application of the model developed by Chmielewski and Potts (1995) accounted for 21% of the variation in observed yields in an independent dataset. This model had only three fitted climate variables – total growing season precipitation, maximum temperature in June and minimum temperature in July (radiation data was unavailable and therefore not included). By contrast, Landau et al. (1998) fitted 17 climate variables, four of which could account for 61% of the variation accounted for and had a physiological explanation.

In this study, the climate effects accounted for considerably less of the total variation explained (11%) than in previous studies. The main climatic effects fitted were; (i) reduction in yield with increased minimum temperature in March, (ii) a negative rainfall effect in January and (iii) a reduction in yield with increased maximum temperature in May. These could be associated with; (i) a reduction in the formation of roots and yield bearing shoots, (ii) waterlogging and/or disease and pest incidence and (iii) negative impacts on yield forming stem reserves and/or deep roots, respectively (HGCA, 2008). The only monthly climate data effects that were selected both in this study and by the comparative previously reported regression models discussed above were maximum temperature in July and minimum temperature in May, from the model of Landau et al. (1998); however, opposite effects on yield were estimated for both these climate-yield responses, with increases in yield observed in this study, whilst negative impacts were fitted in the Landau et al. (1998) model. Both in this study and the previous examples, overall negative effects of rainfall on crop yields were estimated. Chmielewski and Potts (1995) included a negative term for total growing season precipitation as most monthly precipitation variables were significant. Of the five fitted monthly rainfall effects in the model for Landau et al. (1998), four were negative. Both rainfall variables in this statistical model were

negative. A comparison of the climate variables fitted in Landau et al. (1998) reveals that a similar proportion of the variation in yield explained by climate effects could be attributed to rainfall effects, 21% and 26% in this study and that of Landau et al. (1998), respectively. Minimum temperature effects were more dominant in this study, accounting for over half the explained variation accounted for by climate variables; in the Landau et al. study only 19% was attributed to this effect. Maximum temperature effects were more important in Landau et al. (1998) model, accounting for over a third of the variation explained by climate effects, in comparison with only 13% in this study.

Alternative formulations of the empirical model were explored, utilising accumulated versions of the weather variables (rainfall, radiation and thermal time). This resulted in a slightly reduced model performance (r^2_{adj}=0.38). Total growing season radiation and rainfall were not included in this model, although a total thermal time variable (calculated from month minimum and maximum temperatures) was. Under this setup, climate variables became more important, accounting for 54% of the total variation explained. Accumulated rainfall in June was the most important predictor, accounting for 20% of the total variation explained, and having a negative effect on crop yield. Whilst crop protection and spray expenditure remained important to model predictions, accumulated radiation in November was the second most important predictor, having a positive effect on crop yields.

The potential of including observations of soil characteristics was also explored, through consideration of observations describing exchangeable potassium, soil organic carbon, clay and pH in the statistical model during development. Although it is arguable that these observations averaged at this level are not meaningful

(Hoffman et al., 2006). Two variables (exchangeable potassium and pH) were included in the statistical models considered during development, using monthly and accumulated variables, respectively. However they did not alter the overall performance of the empirical model and the amount of variation they explained was negligible (<0.4% and 1%, respectively).

The described differences between Simple-EMP and previous empirical models are unsurprising, as sub-optimal management alters the response of yields to climate (Landau et al., 2000). Deficiencies in management are likely to be more pronounced in the farm environment, than under experimental conditions. The models of Landau et al. (1998; 2000) and Chmielewski & Potts (1995) were developed using optimally-managed trial yields, assumed to be limited only by meteorological variables. However, the dominance of negative rainfall effects in these models suggest that even in these environments, deficiencies in management could be occurring, leading to incomplete control of pests, disease, water-logging and nitrogen leaching. Accounting for these additional sources of variation in yield could improve the yield predictions of such empirical models. This is especially relevant in the UK, where yield variation is less dominated by the (non-marginal) environment (Landau et al., 1998). The empirical model presented here attempts to account for a wider range of influences, through the incorporation of management variables to account for these additional sources of variation; indeed the majority of the yield variation explained was attributed to these management variables. Expenditure on crop protection was the dominant factor affecting yields, supporting the suggestion that the primary impact on yield in many environments may be disease and not nutrient limitation (Jamieson et al., 1999). Although fertiliser expenditure alone did not significantly influence yield, but was included in the model in the crop protection x fertiliser

expenditure interaction; however, fertiliser became the dominant factor if crop protection expenditure was omitted from the regression. These variables may be, in part, a proxy for farm level intensity of production, for example organic or low input system will respectively utilise none and limited inputs of both fertiliser and crop protection; by contrast specialised wheat producers will be arguably more likely to utilise higher levels of both these key inputs.

All significant expenditures (crop protection, land, machinery, contractor, other) result in increased yield in the empirical model. The reduction in yield associated with manure applications could be attributed to the lower yielding organic farms having a greater manure expenditure associated with them (double that of non-organic farms). The presence of organic enterprises on the farms had variable effects on the yields of wheat crops. Higher yields were estimated for farms without any organic enterprises and farms with an organic dairy. The improved yields could be attributed to; (i) specialisation of farms, and (ii) application of nutrient rich manures, respectively. The presence of organic sheep on the farm was estimated to reduce wheat yields, potentially as a result of the absence of associated beneficial manure applications as seen with organic dairy enterprises. Unlike dairy cows, sheep are not usually housed over winter, which prevents the collection of manures produced during this period.

The results indicate a negative relationship between the wheat to fertiliser price ratio and crop yield. Under a market environment in which prices are known and fixed at the outset of production we would expect a positive relationship between these variables. However, despite the use of a wheat futures market, providing a mechanism for farmers to secure a fixed output price either prior to, or during, the

production season, uptake of futures trading by farmers remains lower than initially anticipated (Pannell et al., 2008). Hence during the production season when farmers are applying fertiliser, the output price for the growing crop is largely unknown, and moreover is highly variable. Thus the dynamic nature of farm management decision-making in relation to fertiliser to wheat price ratios may not be adequately captured by within crop production and marketing season interactions.

5.7.2 Simple-MECH Model

Mechanistic models have previously been demonstrated to be excellent predictors of yield variation in winter wheat ($r^2 \geq 0.86$) (Jamieson et al., 1998b). However, previous studies have also demonstrated the importance of fully calibrating such crop models (Landau et al., 1998; Palosuo et al., 2011), which is often difficult to achieve, even at the field scale. A study that used eight mechanistic crop models to simulate observed winter wheat yields across Europe found that if restricted calibration was performed, the models could only explain approximately 1-35% of the variation in observed yields at the field level (Palosuo et al., 2011). Landau et al. (1998) reported that three mechanistic models were unable to satisfactorily predict the observed yields of a large dataset of field trials for which sowing and harvest dates were unavailable and cultivar information was only partially available. This highlights the issues with applying such models at scales larger than the field, where the required detailed input data are not available. Mechanistic models have been demonstrated to perform better under marginal environments, where the effect of climate on yield is stronger (e.g. Challinor et al., 2004). In environments, such as the UK, where climate is not directly responsible for yield variation, the resulting 'noise' in yield data from management deficiencies can result in models performing poorly (Jamieson et al., 1999; Landau et al., 2000; Palosuo et al., 2011).

As in the empirical model, the majority of the mechanistic model's explanatory power could be attributed to inclusion of crop protection and fertiliser effects. Addition of other potential effects only slightly improved the model's ability to account for variation in observed yields. A similar effect of the correlation between crop protection and fertiliser expenditure was noted, with the fertiliser expenditure description producing a model almost as powerful (r^2_{adj}=0.18) as that containing the crop protection description (r^2_{adj} = 0.24), but the combined model was only slightly more powerful (r^2_{adj} =0.26).

The negative effects of increasing rainfall estimated in the empirical model, were also noted in the mechanistic approach. Although addition of a drought effect did not improve the model's explanatory power, damage to the crop (through a loss of biomass) during months of threshold exceeding rainfall did. This only accounted for a small proportion of the variation in yield (1%), but supports the suggestion that physical damage, lodging or increased pest or disease due to rainfall events are reducing yields. Although most mechanistic crop models include effects of nutrient limitation on yield, descriptions of disease or pest effects are rarely included, and they are usually assumed to be non-limiting (Mirschel et al., 2014).

Although mechanistic crop models commonly simulate growth and development on a daily time-step, here a monthly time-step was necessitated by the driving meteorological data. The model could be improved by considering daily meteorological information, as monthly averaging may mask significant effects.

The mechanistic model, which is based on canopy growth over time, is hindered by the lack of data on key timings, such as sowing, harvest and phenology dates, that are typically important in mechanistic models. As noted in the discussion between

Jamieson et al. (1999) and Landau et al. (1998), assumed sowing and phenology dates can have a significant effect on predictions made by mechanistic models, resulting in their inability to simulate yields accurately. In this model, yields on average increased 3.9% and decreased 3.2%, if the sowing date was moved back or forward two weeks, respectively. This indicates that attributing the same sowing date to all farms may account for some of the models inability to reproduce the variability in observed yields. Additionally, the mechanistic model currently only contains two management effects – fertiliser and crop expenditure – and could be developed to include additional descriptions of effects that significantly impacted on yield as determined in the empirical model. For example, a greater farm area (6% of the variation in yield accounted for) could increase the efficiency of application of fertiliser and crop protection to the crop canopy. An analysis of the area of wheat grown by the farms in the survey revealed that the average size was 81.5 ha, but there was a wide range in sizes reported (s.d.=112.9 ha) from a minimum crop wheat area of 0.5 ha to a maximum of 2009 ha.

5.8 Conclusion

To date, modelling of crop yields has largely focused on either the small or large scale, emphasising the prediction of field or regional yields, especially in the face of climate change. Little attention has been paid to estimating farm yields, with a focus on the effects of non-meteorological factors on crop yields, particularly in non-marginal environments such as the UK. The models developed here aimed to address this research gap, utilising accessible data.

Given the food security implications of modelling farm-level yield variation in contrast to modelling experimental yield variation, our results demonstrate that empirical

approaches may provide more appropriate mathematical representations of contemporary primary food production practices than bio-physical representations alone. In the empirical model, Simple-EMP, climate variables accounted for a quarter of the variation in yield explained, with the mechanistic model design, Simple-MECH, unable to simulate the variation in yields without additional management descriptions. Both models were unable to simulate the full range of yields observed. The majority of the variation in observed yields could be attributed to management variables, primarily crop protection and fertiliser expenditure, which were significantly positively correlated.

The empirical approach allows the description of the impact of variables on a farm's yield, whilst the mechanistic model attempts to explain the impact of these variables, by considering the processes driving yield – in this instance canopy and biomass growth as a function of climate, fertiliser and crop protection expenditure. In this research, where the basis of the model formation is monthly and annual data, the empirical approach could be more appropriate – as the results suggest – with the mechanistic approach more suited to modelling using daily input data. Some studies have developed hybrid empirical models to describe wheat yields – with a regression model applied in conjunction with additional descriptions, for example drought (Qian et al., 2009) and phenology (Landau et al., 2000). Landau et al. (2000) simulated the effects of fitted climate effects over five growth phases to explain 17% of the variance in observed yields in an independent test. However, this approach is unsuitable for on farm yields, where for example, detailed phenology or soil water measurements are unavailable.

The FBS dataset contains further detailed farm management statistics, including records on crop proportions that could significantly influence wheat yields. For instance, a key issue in modern wheat cultivation is black-grass – a weed that germinates alongside autumn sown cereals and has developed multiple herbicide resistance – which can significantly reduce yield through competition for light, water and nutrients. This can be controlled by crop rotation using spring-sown crops or fallow or grass ley breaks of more than a year (HGCA, 2014). This could be considered in the future using already available data describing the use of such 'break crops' on the farms surveyed, with the expectation that yield increases would be associated with a greater 'break crop' area planted. In addition, in recent FBS reports, more detailed statistics were collected on the physical quantities of fertiliser used per farm, which could also be incorporated.

Given the food security implications of modelling farm-level yield variation in contrast to modelling experimental yield variation, our results demonstrate that empirical approaches may provide more appropriate mathematical representations of contemporary primary food production practices than mechanistic representations.

6 Discussion

This thesis has presented the development and analysis of crop models of differing complexity, ranging from a simple, static, empirical model, to a relatively complex, dynamic, mechanistic model. The following objectives were addressed:

i. **Can differences in wheat cultivar growth and development at the field level be similarly explained using simplified versions of an existing mechanistic model?**

Application of crop models to climate change prediction has highlighted the limitations of the traditional, complex, mechanistic models and the potential of empirical models at the broader scale. In addition to developing new models, both empirical in nature and simpler, mechanistic models developed with consideration of the larger-scale at which they could be applied, existing models can be simplified to remove redundant processes and parameters, to not only make them easier to apply at the larger-than-field scale, but also to reduce the uncertainty associated with model structure and parameters, and aid in achieving identifiable parameterisations, e.g. for cultivar-specific parameters. An analysis of an existing mechanistic model (Sirius) demonstrated that the cultivar-specific parameter values fitted were subject to the initiating values. This, in addition to a large number of significant correlations between the cultivar-specific parameters, indicated that the model was over-parameterised and thus was a candidate for model reduction.

The reduction analysis performed here expanded on earlier work (Crout et al., 2014), considering model parameters (describing cultivar differences) in addition to model structure in the reduction analysis. The analysis demonstrated that it was not necessary to have all currently considered processes and parameters describing

cultivar differences to maintain model performance. Simplifications could be made to model descriptions and not all cultivar-specific parameters were required. Thus, differences in wheat cultivar growth and development at the field level could be explained using a simplified version of the Sirius model (Sirius-R). This analysis performed for Sirius indicates that there is no value in the un-reduced Sirius in this application, i.e. to predict differences in leaf area, biomass and grain yield for different cultivars under nitrogen trials across sites in the UK and France. Similar results were obtained for the newly developed Intermediate model. There are processes within the models and parameters describing cultivar differences that do not contribute to predictive power in this application. These processes and parameters only add to the complexity of the model, with no associated benefit. This unnecessary complexity is a barrier to application, analysis and understanding in crop models (e.g. Soltani & Sinclair, 2012). However, the reduced models, Sirius-R and Intermediate-R, are a product of the data used to generate them. There is no suggestion that these reduced versions of the model are widely applicable. They are dependent on the quality (e.g. number of crop components, frequency of observations) and focus (e.g. nitrogen trials) of the data used. In this instance, the reduced models developed here could be applied to predict optimal nitrogen fertilisation, but it would not be appropriate to apply them to assess irrigation strategies, as only nitrogen trial datasets were used in the development of these reduced models. The differences in redundancies, as well as differences in replacement values for similarly identified redundant variables, noted between this research and that of Crout et al. (2014), highlight the dependency of model reduction outcome on the data utilised. Both applications considered within season measurements of multiple crop components, although on a limited number of trials.

This model reduction exercise was performed at the field level, the scale at which Sirius was developed and initially applied. Given that at this scale, a number of areas of reduction, particularly with respect to parameters describing cultivar differences were identified, suggest that if the model is applied at broader scales, at which there is argument for a reduced level of detail (e.g. Challinor et al., 2004), there is likely even further potential for reduction. Additionally, given that Sirius is considerably simpler than other mechanistic crop models (e.g. APSIM), the potential for reduction in these more complex models for a given application, which contain a much larger number of parameters, and more numerous, highly detailed, interacting processes is likely substantial.

In light of the above, the following should be considered;

- re-consideration of current approaches to parameter estimation for mechanistic models with parameter identifiability issues – only adjusting cultivar-specific parameters of interest or only adjusting parameters that the model is most sensitive to – with a comprehensive, exhaustive method of automated model reduction
- application of such systematic, automated reduction methods to existing mechanistic models, to identify redundant model parameters and processes for a given application, e.g. here, to predict differences in cultivar growth and development under varying nitrogen applications
- the application of the reduced model, as this needs to inform the data used in the reduction, and ensure the appropriate modelled processes and parameters will be tested, e.g. here, within-season growth and development observations for nitrogen trials with multiple cultivars, to assess the

performance of simulated growth and development of the cultivars (as described by differing parameters) throughout the season

ii. What modelling approach (empirical or mechanistic) is suited to modelling yield at the farm scale using farm-level observations?

In contrast, to the more complex, field-scale models discussed above, developed and applied using relatively detailed field-level observations, two new simpler models, an empirical (Simple-EMP) and a mechanistic model (Simple-MECH), were developed using relatively coarse farm-level observations. These models were developed to predict yields at the farm level, did not consider cultivars, or developmental processes, instead focusing on end-season yield prediction for winter wheat. These simple models – a statistical and mechanistic model – were developed using nationally collected monthly meteorological observations and annual farm management information collected for official statistics.

The resulting empirical model was able to explain a greater proportion of the variation in observed yields (41%) than the mechanistic model (25%), appearing to be a better approach at this scale, which required the model to be driven by datasets of monthly and annual observations, which lacked information regarding key timings of sowing, harvest and fertiliser application dates. This makes it challenging to apply a dynamic, mechanistic model (Jamieson et al., 1999; Landau et al.. 1998). Application of the relatively complex, mechanistic Intermediate Model (Chapter 4), for example, at the farm-level required an even larger number of assumptions to be made, and the yield predictions were less accurate than the simple models. Thus, a simpler mechanistic model, formulated with an appropriate level of details for the

scale of interest and the data available, has the potential to out-perform a more complex one, developed for use at a different scale.

Additionally, the empirical model was able to incorporate a number of management effects that the mechanistic model did not consider, but were found to have a significant effect on yield, for example, farm area. Although the empirical model appears better suited to modelling yield at the farm scale using farm-level observations, it has been argued that the differences in the data requirements, sensitivities of empirical and mechanistic models makes it advantageous to consider both approaches, for a more complete understanding (Estes et al., 2013a; Estes et al., 2013b; Watson et al., 2015; Morin & Thuiller, 2009; Giardin & Tardif, 2008). In this application, both models attributed the majority of their explanatory power to crop protection and fertiliser and both included a negative effect of rainfall. In the mechanistic model, this negative rainfall effect was simulated as a loss of biomass through damage in months in which rainfall exceeded a threshold, which was also identified by the statistical model, as negative yield effects associated with rainfall in January and June. Although the empirical model is capable of describing the negative effect of rainfall associated with these months, the formulation of the mechanistic model offers a potential explanation for this effect.

The FBS survey is an excellent, on-going, potential data source for the formation, and improvement, of crop models at the farm-level. The information is collected annually, with statistics collected for both arable and pastoral farms. Thus, this approach could be extended to consider other crops. There are further statistics that would be interesting to consider incorporating into the models, for example, break-crop area records as a proxy for weed control, or the percentage of a farm within a

Nitrogen Vulnerable Zone, and any impact this might have on the application of fertilisers (FBS, 2017).

At model development, only five years worth of FBS data was available for research purposes (2005-2010). Currently there could be up to another seven years worth of statistics available to further develop and test the model. Further, additional statistics are now being collected that are more relevant to traditional crop modelling, e.g. fertiliser quantities per hectare (FBS, 2017). This would remove the necessity of using expenditure as a proxy for fertiliser application and could improve the applicability of the mechanistic model, in particular. In addition, model performance could be improved by utilising daily rainfall data, which is now generally available, but was prohibitively expensive at the time of this research (*N.Crout, pers. comm.*). Monthly averaging may mask extremes, which could now be considered.

Collection of FBS data is on-going and collaboration with the modelling community could direct the addition of data that would be useful in the further development of the yield models. One particular assumption that was made commonly in both models, was the sowing and harvest dates of the winter wheat crop across all farms. Addition of simple timing statistics like this, that are typically important in mechanistic models, could improve predictive power, enabling the model to better reproduce the variability in yields.

In summary:

- An empirical model approach appeared more suited to modelling at the farm-scale, than a mechanistic approach, being able to explain a greater proportion of the variation in farm yields

- Application of this empirical approach alongside a mechanistic approach, however, could allow explanations of effects identified in the descriptive, empirical model
- A mechanistic model, of intermediate complexity developed for application at the field-scale using field level data, also performed poorly when applied at the farm-level, due to the large number of assumptions that had to be made

In light of the above, the following future work is identified:

- Update of the empirical and mechanistic models developed here, with the aim of improving the predictive power of both models, by:
    - utilising the additionally available annual statistics (2011-)
    - incorporating fertiliser quantities per hectare, rather than using fertiliser expenditure as a proxy (for the years this is available)
    - exploring the use of variability available in daily rainfall data across the month to incorporate the effect of minimum/maximum and/or extreme values, to identify whether consideration of these values can improve model predictive power
    - collaborating with the FBS to collect additional, key timing statistics, important in effective crop model application – suggested here are sowing and harvest dates for farms

A further important consideration when modelling systems is the computational time required for evaluation and analysis of models. The run-time differed considerably between the complex, intermediate and mechanistic simple models. When considering the multi-cultivar dataset, the more complex model took considerably

longer to compile (translate the coded model into computer code in preparation for execution of the model) and evaluate than the simple and intermediate models (Table 6.1). Although these times do not constrain the complex model for single point use, they quickly become challenging for iterative analyses, such as are employed in model parameterisation and reduction.

Table 6.1 Mechanistic Model Complexity Comparison

Model	Total Variables	Total Parameters	Total Cultivar Specific Parameters	Redundant Variables	Module Number	Computation Time (seconds)
Sirius	435	42	11	6	33	15
Sirius-R	429	35	4	-	33	-
Intermediate	151	31	12	6	15	0.9
Intermediate-R	146	25	4	-	15	-
Simple-MECH	62	14	-	-	2	0.1

7 Summary

- The existing mechanistic model (Sirius) and newly developed intermediate mechanistic model (Intermediate) were both found to be over-parameterised during parameter estimation for 16 wheat cultivars at the field level
- The new intermediate model produced predicted grain yield, biomass and anthesis date with similar accuracy to the complex model, although the simulation of LAI was much poorer
- Reduction analyses were performed for both Sirius and the Intermediate model to identify model variables (or processes) and cultivar-specific parameters that were redundant and could be replaced with a fixed constant, generating the Sirius-R and Intermediate-R models

- Only a small number of variables were identified as redundant, however the number of cultivar parameters estimated could be substantially reduced in both models, without detriment to predictive ability
- These reduced models (Sirius-R and Intermediate-R) are a product of the data used for the reduction analyses, and thus their application is to predict growth and development of differing cultivars under differing levels of nitrogen fertilisation
- Two simple models – an empirical (Simple-EMP) and mechanistic model (Simple-MECH)– were developed for predicting farm level yields of winter wheat
- The empirical model performed better at the farm level, with the mechanistic model hindered by the coarse observation detail
- The farm survey data used to develop the Simple-EMP and Simple-MECH is collected annually, and there is already potential to develop these models further

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2.10 Method Summary

Chapter	Objectives	Datasets Used	Tools Used

3	To assess the ability to parameterise, and parameterise, an existing, complex wheat model for multiple cultivars using field level observations
	
	Identify potentially redundant processes in this complex model using a reduction analysis
		NUE Trial (Multi-cultivar)	• Metropolis-Hastings Parameterisation
			  ○ Multiple independent rounds (4) to assess identifiability
			• Parameterisation Analysis:
			  ○ Sensitivity analysis
			  ○ Correlation
			• Model Reduction
			  ○ Variables
			  ○ Cultivar parameters

4	To develop, parameterise and analyse for reduction, a model of intermediate complexity using field level observations
	
	Investigate the application of this intermediate model to farm-level yield prediction
		Nitrogen and Drought Trials (Single-cultivar)
		
		NUE Trial (Multi-cultivar)
		
		FBS Farm Survey
			• Metropolis-Hastings Parameterisation
			• Parameterisation Analysis
			• Model Reduction
			  ○ Variables
			  ○ Cultivar parameters

5	To develop, parameterise and validate both a simple empirical and a simple semi-empirical, bio-physical model of wheat using farm level observations	FBS Farm Survey	• Model Development:
			  ○ Metropolis-Hastings Parameterisation
			  ○ Stepwise Regression