Sexton, Justin David (2015) ***Bayesian statistical calibration of variety parameters in a sugarcane crop model.*** **MSc thesis, James Cook University.**

Bayesian Statistical Calibration of Variety Parameters in a Sugarcane Crop Model

Thesis submitted by

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In partial fulfilment of the requirements for the
degree of Masters by Research (Mathematics) in the
College of Science, Technology and Engineering,
James Cook University, Townsville

Thesis submitted:

April 2015

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Acknowledgements

At this time I would like to acknowledge and thank my thesis supervisors Dr. Yvette Everingham and Dr. Geoff Inman-Bamber for their support encouragement and insight, without which this work could not have been accomplished.

I would like to acknowledge and thank Dr. Jaya Basnayake, Dr. Prakash Lakshmanan and Dr. Philip Jackson for supplying the sugarcane breeding trial data from the More Crop Per Drop (BSS334) project funded by the Sugar Research and Development Corporation (now Sugar Research Australia). I would also like to thank Dr. Michael Robertson for his help in obtaining field trial data used in the final chapter of this thesis and Dr. Peter deVoil and Dr. Bangyou Zheng for their assistance with technical aspects of the APSIM, software.

Finally I would like to thank my parents and family for all their support over the last two years.

Statement on the Contribution of Others

Dr. Yvette Everingham, Senior Lecturer, College of Science, Technology and Engineering, James Cook University and Dr. Geoff Inman-Bamber, Adjunct Research Fellow, College of Science, Technology and Engineering, James Cook University supervised this thesis helping to develop the original proposal as well as providing editorial assistance throughout the thesis. Dr. Yvette Everingham provided mathematical and statistical expertise and support while Dr. Geoff Inman-Bamber provided expertise and support in sugarcane physiology and crop modelling. The comments of two examiners were provided editorial assistance throughout the thesis.

Sugar Research Australia Limited (ABN 16 163 670 068) provided a stipend of $30,000 per year as well as an operating budget of $10,000 per year for the two year duration of the thesis. The project was funded as SRA project STU076. James Cook University provided $1,500 per year for project support as part of the university's "Minimum Resources Policy" for higher degree research students.

Editorial assistance for the first draft of Chapter 1 was supplied by Dr. Everingham and Dr. Inman-Bamber, Dr. Philip Jackson (Principle Research Scientist at the Commonwealth Scientific and Industrial Research Organisation (CSIRO)), Dr. Prakash Lakshmanan (Manager, Sugar Research Australia) and Dr. Jayampathi Basnayake (Senior Researcher, Sugar Research Australia). Editorial comments of the first draft helped to define the overall scope of Chapter 1.

The research question of Chapter 2 was developed with input from Dr. Everingham and Dr. Inman-Bamber. The data for the Home Hill field trial simulated in Chapter 2 were supplied by Dr. Basnayake on behalf of the More Crop Per Drop project funded by the Sugar Research and Development Corporation as project BSS334. The range of values for the transpiration efficiency parameter used in the sensitivity analysis of Chapter 2 was based on pot trial data supplied by Dr. Jackson. Dr. Inman-Bamber provided original simulation files used to model the field trial data and provided assistance with interpreting simulation output. Editorial assistance was supplied by Dr. Basnayake, Dr. Everingham, Dr. Inman-Bamber, Dr. Lakshmanan and Dr. Jackson.

Dr. Everingham assisted in developing the research question of Chapter 3 as well as supplying editorial assistance. Data from the field trial used in Chapter 2, (supplied by Dr. Basnayake) were used to develop the APSIM-Sugar simulation files used in the analysis performed in Chapter 3.

The observed data also help develop the prior distributions for several parameters (number of green leaves, radiation use efficiency and root conductance). The prior distribution for the transpiration efficiency parameter was based on data supplied by Dr. Jackson. Dr. Inman-Bamber identified parameters to include in the sensitivity analysis of Chapter 3 that were not considered variety specific in the literature and provided the methodology for developing the prior distributions for parameter values.

The data for field trials simulated in Chapter 4 and original simulation files were supplied by Dr. Michael Robertson (Deputy Chief; Ecosystem Sciences, CSIRO). Dr. Everingham and Dr. Inman-Bamber contributed to the development of the research question for Chapter 3 and provided editorial assistance. Dr. Bangyou Zheng (Postdoctoral Fellow, CSIRO) provided assistance with generating simulation files using the R statistical program. Dr. Peter deVoil (Senior Research Scientist, Department of Agriculture, Fisheries and Forests, Australia) provided assistance with running simulations on a high performance computer cluster run by the Agricultural Production Systems Research Unit.

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Abstract

Process-based agricultural systems models capable of simulating crop growth, management decisions and varietal differences in productivity allow researchers to investigate the interactions between varieties, production environments and management decisions. The Agricultural Production Systems sIMulator (APSIM) currently includes variety parameters that represent physiological traits for 14 sugarcane varieties. Unfortunately most of these 14 sugarcane varieties are no longer grown commercially. This makes it difficult for industry decision makers to trust the outputs from the model and thereby incorporate model outputs into the decision making process. To overcome this weakness in the APSIM crop model for Australian sugarcane systems the following thesis objectives were developed:

1. investigate the capability of the APSIM-Sugar model to simulate yield differences between sugarcane varieties under different climatic conditions;
2. investigate the sensitivity of model outputs such as biomass and sucrose yields to key model input parameters; and
3. evaluate the use of two Bayesian approaches to calibrate variety parameters in the APSIM-Sugar model.

The APSIM-Sugar model was used to simulate biomass and sucrose yields of four sugarcane varieties grown under well irrigated and water stressed conditions in a breeding trial conducted at Home Hill, Queensland, Australia. Comparisons were made between observed and simulated varietal differences in yield and yield response to water stress. Bayesian Analysis of Computer Code Output (BACCO) was then used to perform a global sensitivity analysis of model outputs (biomass and sucrose yields) to key variety parameters under well irrigated and water stressed conditions. Finally, Generalized Likelihood Uncertainty Estimation (GLUE) and Markov Chain Monte Carlo (MCMC) techniques were used to calibrate APSIM-Sugar influential variety parameters. GLUE and MCMC were evaluated based on a theoretical and real world calibration. APSIM-Sugar was able to accurately reproduce the average biomass and sucrose yields of the four sugarcane varieties grown in the Home Hill trial when effects of weeds, lodging and stalk death were implemented in the simulation. However, APSIM-Sugar had limited skill in simulating yield differences between varieties and varietal yield responses to water stress. Global sensitivity analysis identified how key APSIM-Sugar input parameters affected model outputs. Parameters representing radiation use efficiency (*rue*), transpiration efficiency (*transp_eff_cf*), number of green leaves (*green_leaf_no*) and the leaf size profile (*leaf_size*) were found to strongly influence simulated biomass and sucrose yields. In a real world application, the MCMC calibration of Australian variety Q117 was better able to reproduce observed yields than the GLUE calibration and was able to estimate realistic parameter values for difficult to measure traits such as transpiration efficiency, using readily available field data.

Results from this thesis clearly show that updated variety definitions are needed for APSIM-Sugar. This thesis developed and tested a methodological framework which include performing a global sensitivity analysis and a Bayesian approach to calibrate variety parameters in APSIM-Sugar. The methodological framework provided a validated strategy for improving and updating variety definitions.

Several avenues for future research into the simulation of variety, environment and management interactions in sugarcane systems were identified in this thesis. The comparison of simulated and observed differences between sugarcane varieties highlighted a clear and pressing need for improved and updated variety definitions in current sugarcane models such as APSIM-Sugar. Variety parameters in the APSIM-Sugar module can now be routinely updated as new varieties are released using a limited amount of data which is collected in breeding programs and the methodological framework implemented in this thesis. Updating the model to include variety definitions for current commercial varieties will allow industry decision makers to have greater confidence in the model outputs.

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Publications

Chapter	Details of publication(s)	Status
2	Sexton, J., Basnayake, J., Everingham, Y., Inman-Bamber, G., Lakshmanan, P., Jackson, P., 2014. Detailed trait characterisation is needed for simulation of cultivar responses to water stress, Proceedings of the Australian Society of Sugar Cane Technologists: Gold Coast, Queensland, Australia.	Published
3	Sexton, J., Everingham, Y., 2014. Global sensitivity analysis of key parameters in a process-based sugarcane growth model - A Bayesian approach, In: Ames, D.P., Quinn, N.W.T., Rizzoli, A.E. (Eds.), Proceedings of the 7th International Congress on Environmental Modelling and Software: San Diego, California, USA.	Published
4	Sexton, J., Everingham, Y., Inman-Bamber, G., 2015. A dual method evaluation of the use of two Bayesian techniques for the calibration of variety specific trait parameters in a sugarcane crop model. Environmental Modelling & Software*,* (submitted).	Submitted

Thesis Overview

This thesis had three main objectives:

1. to investigate the capability of a sugarcane crop model to simulate yield differences between sugarcane varieties under different climatic conditions;
2. to investigate the sensitivity of model outputs such as biomass and sucrose yields to key model input parameters; and
3. to evaluate the use of two Bayesian approaches to calibrate variety parameters in a sugarcane crop model.

The ‘Sugar’ module in the Agricultural Production Systems sIMulator (Keating et al., 1999) was the crop model used and is referred to throughout the thesis as APSIM-Sugar. Figure 1 provides a flow diagram of the thesis.

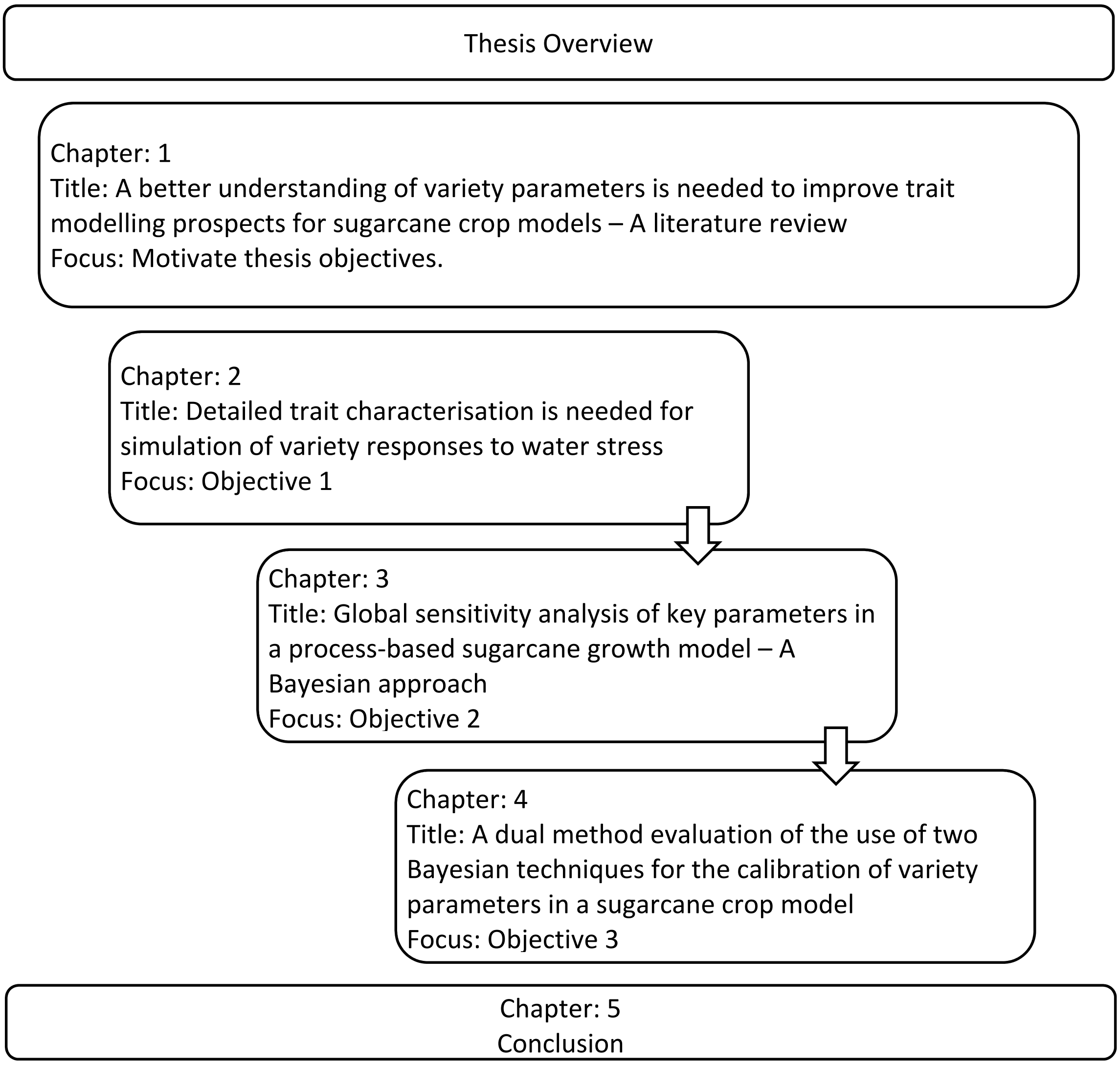

Figure 1. Flow diagram of thesis chapters

The objectives of this thesis required inter-disciplinary solutions that integrated sugarcane physiology and agronomy, sugarcane crop models and statistical sensitivity analysis and model calibration techniques. The literature review presented in Chapter 1 broadly introduced these concepts and motivated the objectives of the thesis which were then explored in subsequent chapters.

Chapters 2, 3 and 4 addressed objectives 1, 2 and 3 respectively. The capability of the APSIM-Sugar model to simulate varietal differences was investigated and included as Chapter 2. Here observed and simulated yields for four sugarcane varieties were compared, illustrating the need for a better understanding of how varieties are represented in the model. The sensitivity of simulated biomass and sucrose to key parameters in the APSIM-Sugar model was then investigated (Chapter 3). The specification of prior parameter distributions and the identification of influential and uninfluential variety parameters presented in Chapter 3 were critical to the application of Bayesian statistical parameter estimation techniques presented in Chapter 4. Identifying influential and uninfluential parameters reduced the number of parameters that needed to be calibrated, improving the efficiency of the calibration techniques. Finally, the Generalized Likelihood Uncertainty Estimation (GLUE) and Markov Chain Monte Carlo (MCMC) calibration techniques were used to calibrate the variety parameters of APSIM-Sugar in a theoretical and real world evaluation (Chapter 4). Chapter 5 was written as a conclusion to the thesis, bringing together the key findings from Chapters 2, 3 and 4.

Chapters 1 to 4 were structured in the format of stand-alone papers. Chapter 2 was based on a published, peer reviewed conference paper under the title “Detailed trait characterisation is needed for simulation of cultivar responses to water stress” (Sexton et al., 2014) and results were presented at the 36th Conference of the Australian Society of Sugar Cane Technologists (28th April – 1st May 2014, Gold Coast, Queensland, Australia). Chapter 2 was revised after examination to align better with the stated objectives of the Thesis. This did not change the overall conclusions of the chapter. Chapter 3 was also published as a peer reviewed conference paper under the title: “Global sensitivity analysis of key parameters in a process-based sugarcane growth model - A Bayesian approach” (Sexton and Everingham, 2014) with results presented at the 7th International Congress on Environmental Modelling and Software (15th – 19th June 2014, San Diego, California, USA). Chapter 5 was submitted for publication to the Journal of Environmental Modelling and Software on 27th February 2015 as “A dual method evaluation of the use of two Bayesian techniques for the calibration of variety specific trait parameters in a sugarcane crop model" (Sexton et al., 2015). The greatest advantage of this structure is that each chapter can be read independently without assuming the reader has read the previous chapters. In later chapters, earlier chapters that explain certain analysis in more detail are referenced. Each chapter concludes with a summary of the chapter for ease of reference. Summaries for Chapter 2, 3 and 4 were based on the paper abstracts.

The comparison of simulated and observed differences between sugarcane varieties presented in Chapter 2 highlighted the need for improved and updated variety definitions in current sugarcane models such as APSIM-Sugar. Chapters 3 and 4 describe and validate a strategy to use global sensitivity analysis and Bayesian calibration techniques to make these improvements and updates. This type of approach to improving varietal simulations has not previously been applied to the APSIM-Sugar model. Using the methodological framework described in this thesis the sugarcane industry can calibrate the APSIM-Sugar model for new varieties as they are developed in breeding programs.

Chapter 1

A better understanding of variety parameters is needed to improve trait modelling prospects for sugarcane crop models – A review of the literature

1.1. Introduction

Sugarcane production of the top 10 producing countries in the world ranged from 31.8 million tonnes (Philippines) to 739 million tonnes (Brazil) in 2013 (FAO, 2013). In the same year sugarcane contributed to a total ethanol production estimated at 32.5 billion litres in Brazil (Azadi et al., 2012). Sugarcane production will become more important as society strives to feed and fuel a global population that now exceeds 7 billion and is predicted to exceed 9 billion by 2040 (United Nations, 2013). To meet these demands sugarcane industries have worked continuously to increase sugarcane productivity.

Sugarcane is thought to have two centres of origin, the New Guinea and India-Burma-China regions (Sleper and Poehlman, 2006). The so called 'Nobel canes' (*Saccharum Officinarum*) cultivated in the gardens of New Guinea represents some of the earliest results of selective breeding in sugarcane. It is believed these canes were selected and grown from wild varieties for their large size, bright colours and sweet, chewable flesh. Before breeding programs were designed, yield improvements were achieved by importing new canes from the New Guinea and India-China regions. Sugarcane breeding programs (Figure 1.1**)** were then initiated quickly around the world (Java, British Guiana, Reunion (1889); Queensland (1890); Mauritius (1891); Hawaii (1904); India (1912); Puerto Rico (1913); Florida (1918); South Africa (1929); Mexico (1943)) (Stevenson, 1965).

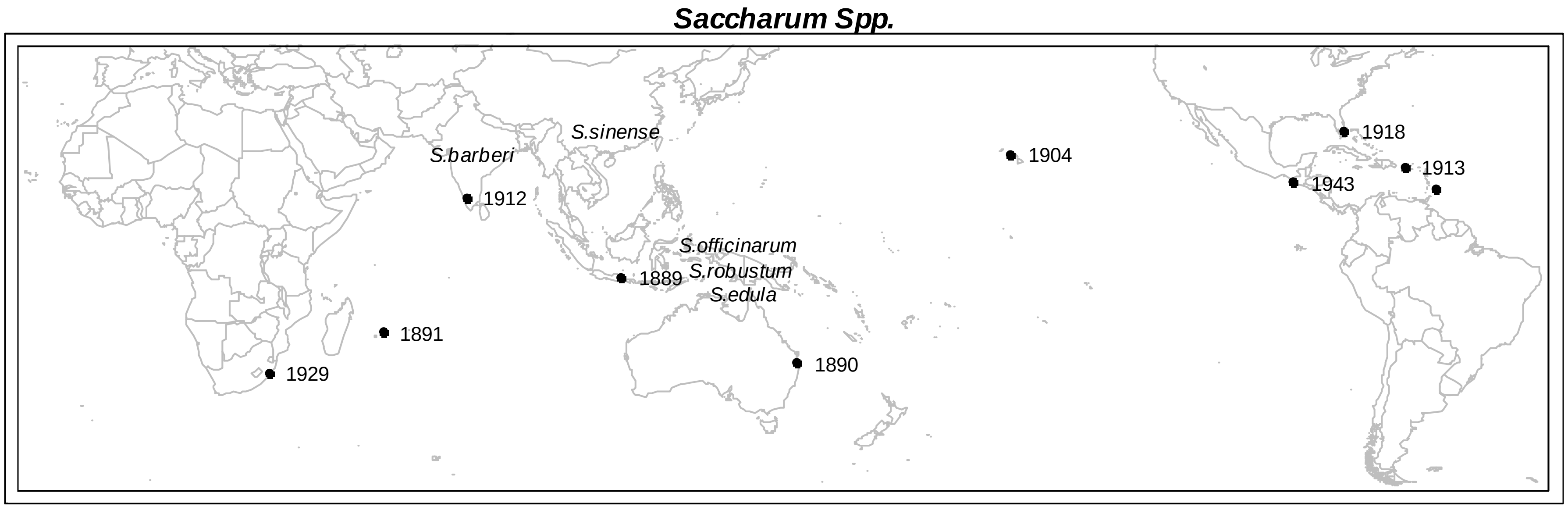

Figure 1.1. Global sugarcane species and first breeding stations. Data adapted from Stevenson (1965)

There are two vital types of breeding programs: nobelization and introgression. Nobelization aims to improve sugar yield through crosses with the Nobel canes (*S. Officinarum*). Introgression programs are the main source of genetic diversity within the breeding population. These programs seek to improve crop resilience through crosses with 'wild' sugarcane species such as *S. Spontaneum* or related genera of the sugarcane complex: *Erianthus, Miscanthus, Narenga and Sclerostachya* (Amalraj and Balasundaram, 2006; Bakker, 1999; Sleper and Poehlman, 2006). Figure 1.2 outlines a standard breeding program in Australia (Hogarth and Allsopp, 2000). A breeding program begins with a bi-parental cross. Computer software and well documented records of crossings can be used to determine optimal crosses by accounting for the agronomic performance and disease resistance of each parent. This process can take up to 12 years before a new variety is released.

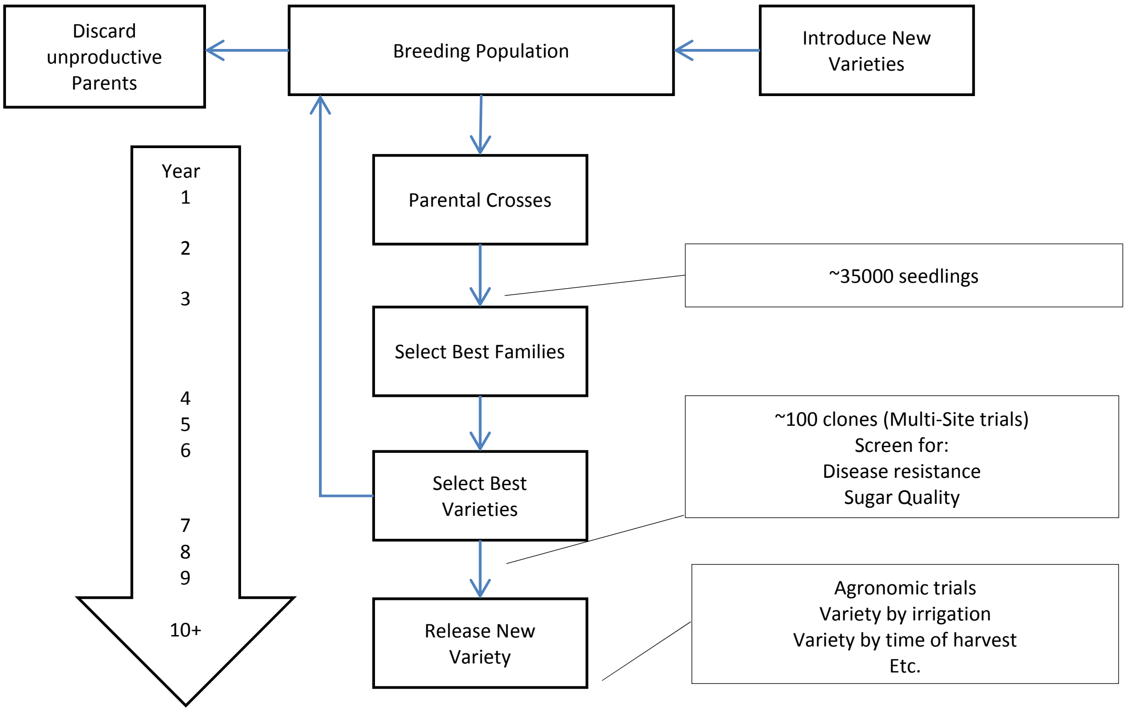

Figure 1.2. Generalised breeding program (adapted from Hogarth and Allsopp (2000)) from an initial bi-parental cross thousands of seedlings are grown in replicated "family" plots. Family plots are harvested and the top producing families (approximately 40%) are retained in the program. Selection continues until a relatively small number of varieties are retained (approximately 150). At this point the reduced set is replanted at multiple sites to assess performance under a range of climatic conditions.

There are many contributing factors to the improvement of sugarcane productivity. The appropriate choices of variety and management strategies for a given environment have been used to increase sugar yields (Singels et al., 2005a; Singels et al., 2005b). Breeding new varieties has also contributed to increased sugar yield (Jackson, 2005) and improved disease resistance

(Wang et al., 2013). While crop models are not widely used to influence sugarcane breeding programs for variety development, there are many examples of sugarcane models investigating management decisions such as irrigation (Inman-Bamber et al., 2006; Everingham et al., 2008), fertilization (Attard et al., 2008) and harvest and plant scheduling (Bezuidenhout et al., 2002; Stray et al., 2012).

Here the term crop model is used to refer to process-based crop models. These models incorporate the current understanding of crop physiological processes (Lisson et al., 2005). Several sugarcane crop models have been developed. Examples include the 'Sugar' module (Keating et al., 1999) in the **A**gricultural **P**roduction **S**ystem s**IM**ulator (**APSIM**; (Holzworth et al., 2014)), the Canegro model (Singels et al., 2008) in the **D**ecision **S**upport **S**ystem for **A**grotechnology **T**ransfer (**DSSAT**; (Jones et al., 2003)), Sugarcane in Agro-IBIS (Cuadra et al., 2012), QCANE (Liu and Bull, 2001), AUSCANE (Jones et al., 1989) and WaterSense (Inman-Bamber et al., 2007). Models such as APSIM-Sugar and DSSAT-Canegro are capable of accounting for environmental conditions such as climate and soil properties, management practices such as irrigation, fertilization, crop rotation and harvest scheduling and variations of traits between varieties of sugarcane. A trait may be defined as any variation of an observable (phenotypic) characteristic such as morphology (e.g. height, stalk diameter, root length etc.), phenology (developmental stages) or process-based physiology (e.g. photosynthesis, respiration, transpiration and water use efficiency).

Crop models that can effectively simulate differences between varieties, allow researchers to investigate the effects of variety on productivity and genetic, environment and management interactions. Specifically, they allow researchers to investigate how varieties have changed over time, identify varieties that will perform well in a given environment, develop management strategies for a given variety, and identify artificial ideotypes for a given or future environment (Jeuffroy et al., 2006). Crop models are also increasingly being used to investigate variety development opportunities in a range of commercial crops including sorghum (Chapman, 2008), wheat (Laurila et al., 2012), soybeans (Boote et al., 2003), peanuts (Putto et al., 2013) and peaches (Quilot et al., 2012). Inman-Bamber et al. (2012) used APSIM-Sugar to simulate the effects of changes in rooting depth, intrinsic transpiration efficiency, and leaf and stalk senescence to biomass yield under well irrigated and water-limited conditions.

To simulate varietal differences it is necessary to calibrate model parameter values that represent crop traits. These values can be difficult to measure directly and are often estimated by comparing simulated yields with observed data. Several statistical methods exist to calibrate model parameters (Makowski et al., 2006a). These techniques often require an understanding of how input parameters influence model outputs in order to reduce the number of parameters that need to be estimated. Sensitivity analysis (Saltelli et al., 2008) allows researchers to quantify uncertainty in model outputs due to model input parameters and has become a standard part of model development and evaluation (Dzotsi et al., 2013; Monod et al., 2006; Wang et al., 2005). This chapter considers how sugarcane models represent varietal differences and the statistical tools such as sensitivity analysis and calibration techniques that can be used to improve the calibration of sugarcane models.

1.2. Sugarcane Crop Models

1.2.1. Advantages of simulating trait differences between sugarcane varieties

Crop models can largely be defined as either empirical (statistical) or process-based models (Singels, 2013). Empirical models simulate crop yields by developing statistical relationships between yield and a relatively small number input parameters. Jiao et al. (2005) developed an empirical model of Commercial Cane Sugar (CSS), a productivity measure used in Australia. Jiao et al. (2005) were able to maximize CCS gains by suggesting improved harvest scheduling. Statistical models have also been used to estimate sugar yields from water use (Kingston, 1994), forecasting yields from time series data (Verma et al., 2013) and explore potential and actual yields based on climate and crop management (Monteiro and Sentelhas, 2014). Process-based models such as APSIM and DSSAT simulate the underlying physiological processes and their interaction with climate variables. This requires a large number of parameters. The complexity of process-based models can lead to a low adoption rate (Everingham et al., 2006; Inman-Bamber et al., 2006; Jakku et al., 2007). However, the relative simplicity of statistical models comes at the cost of potentially misleading assumptions (Lobell, 2013). In both cases it is necessary to understand the effect of errors and assumptions on model accuracy (Watson et al., 2014).

Process-based models can assist in better understanding interactions between varieties, environments and management decisions making them a potential tool in breeding programs.

This potential has not been sufficiently explored for sugarcane. This can be seen in the publication of Singels (2013). In a chapter overviewing sugarcane crop models, Singels (2013) identifies environmental characterization (identifying target environments), trait dissection (identifying genes or quantitative trait loci, QTL that correspond to traits) and trait effect assessment and ideotype design (identifying desirable traits for specific environments) as areas for crop modelling to support crop improvement.

A major concern for the improvement of sugarcane varieties is the apparent slow-down of improvement in sugar yield. Although sugarcane variety improvement has led to yield increases (Lingle et al., 2009; Zhou, 2013b; Zhou, 2013a) the rate of improvement has decreased (Jackson, 2005; Lingle et al., 2010). By reviewing previous studies Jackson (2005) concluded that there had been relatively little increase in sucrose content (measured as CCS) among released varieties in Australia over the previous four decades. Lingle et al. (2010) compared varieties from 7 generations of a Louisiana, U.S.A breeding program (1930 to 2006) and found that juice quality and sucrose yield had plateaued over the last 3 generations (approx. 1980 to 2006). It may be possible to investigate the causes behind the evident slow-down in sugar yield improvement by identifying morphological or physiological traits that could be selected from clones (varieties being developed) that have been overlooked because of a poor set of other traits and low yields. For example, by calibrating the CROPGRO-Soybean model (Boote et al., 1998) for old and new varieties of soybean, Boote et al., (2001) identified that higher photosynthesis and improved partitioning had likely contributed to the historical increase in yields.

Crop models have been used to characterize target growing environments for breeding programs, based on simulated levels of water stress for sorghum (Chapman et al., 2002), maize (Chauhan et al., 2013) and wheat (Chenu et al., 2013). Chapman et al. (2002) used the APSIM-Sorghum model (Hammer et al., 1996) to define target environments for breeding based on patterns of water stress (mid-terminal, severe-terminal and mid-season). The identified environment types were later used to simulate a breeding program by linking the APSIM-Sorghum model and a quantitative genetics model (QU-GENE; (Podlich and Cooper, 1998)) (Chapman et al., 2003). Chapman et al. (2003) found that simulated early maturing varieties were favoured in severe-terminal stress environments while late maturing varieties were favoured in mild-terminal and mid-season stress environments. Patterns of stress are particularly important for sugarcane. Although excessive stress can reduce biomass yields irrigation is intentionally withheld late in the season to increase sucrose juice quality and quantity.

The work of Inman-Bamber et al. (2012) is one of the few published examples of the use of a sugarcane crop model to explore the effects of modifying sugarcane traits for a particular environment. The impact of modifying model parameters related to rooting depth, transpiration efficiency, leaf and stalk senescence and conductance was investigated for the simulation of a water stressed environment. Leaf and stalk senescence did not improve productivity in stressed environments while increased rooting depth improved dry biomass by up to 21% depending on environment and soil conditions.

Part of the underlying physiology a process-based crop model must simulate is the crops developmental phases. Commercial crops such as wheat, sorghum and legumes rely on determinant flowering or reproductive phases. In comparison sugarcane is considered a vegetative crop and reproductive phases are ignored in commercial production. The difficulty in studying and simulating the impact of environmental conditions on vegetative growth compared to fruit or seed development has contributed to the lack of progress in trait simulation in sugarcane. Before progress can be made in simulating varietal differences in sugarcane more detailed research is needed to identify how process-based sugarcane models deal with or define varieties.

1.2.2. How process-based models define sugarcane varieties

Two widely used process-based sugarcane models are APSIM-Sugar and DSSAT-Canegro. Both models have been well validated in the literature (Keating et al. (1999) for APSIM-Sugar and Singels et al. (2008) for DSSAT-Canegro). Both models have been calibrated for a relatively small number of sugarcane varieties (see Cheeroo-Nayamuth et al. (2000) for APSIM-Sugar and Marin et al. (2011) for DSSAT-Canegro). As two of the most widely used models, both have been extensively compared in the literature (Lisson et al., 2005; O'Leary, 2000; Singels, 2013). O'Leary (2000) reported coefficients of determination (r^2) for biomass and sucrose simulation as 0.73 and 0.78 respectively for APSIM-Sugar and 0.73 and 0.66 for DSSAT-Canegro. While there seems to be little difference in the accuracy of the two models, the differences in modelling philosophy are not trivial especially in the context of simulating varietal differences.

APSIM-Sugar and DSSAT-Canegro have similar approaches to phenology, canopy expansion and biomass partitioning (Lisson et al., 2005). In the APSIM-Sugar module, physiological processes and their rate coefficients or parameters are divided into species parameters that are not considered to vary much between varieties, parameters that are specific to plant or ratoon crops and parameters that are specific to varieties within the crop class (plant or ratoon; Table 1.1). DSSAT-Canegro, following DSSAT convention describes parameters as species, ecotype and cultivar (variety) specific parameters (Table 1.2).

Variety parameters for APSIM-Sugar defined in Table 1.1 control canopy development (*leaf_size*, *leaf_size_no*, *green_leaf_no*, *tillerf_leaf_size* and *tillerf_leaf_size_no*); biomass partitioning to cane and sucrose (*cane_fraction*, *sucrose_fraction_stalk*, *stress_factor_stalk*, *sucrose_delay*, *min_sstem_sucrose*, *min_sstem_sucrose_redn*) and developmental stages (*tt_emerg_to_begcane*, *tt_begcane_to_flowering*, *tt_flowering_to_crop_end*). Some physiological traits are represented by single parameters such as thermal time required between emergence and beginning of stalk growth (*tt_emerg_to_begcane*) or senescence induced by ageing which is controlled by allowing only a fixed number of green leaves (*green_leaf_no*). Other physiological traits are represented by combinations of parameters such as the leaf size profile which is defined by the *leaf_size* parameter (area of fully expanded leaf) and *leaf_size_no* (leaf position along the stalk). For simplicity some physiological traits are not modelled explicitly but their effects are included through surrogates. In APISM-Sugar tillering is not directly modelled. Instead, the increased leaf area due to tillering is included by modifying the leaf size profile using *tillerf_leaf_size* and *tillerf_leaf_size_no* parameters (Keating et al., 1999). Currently varieties defined in APSIM-Sugar vary only in leaf size profile and in the partition of biomass to sucrose (Keating et al. 1999).

Table 1.1. APSIM-Sugar variety parameters: Parameters represent morphological traits such as the leaf size profile and number of green leaves, developmental stages or physiological traits. Some traits are described using combinations of variables such as the leaf size profile which is described using parameters *leaf_size* and *leaf_size_no*.

Parameter	Description	Units
leaf_size	Size of each leaf (leaf number 1 to approx. 40) serving as inflection points for leaf size curve	mm^2
leaf_size_no	Leaf number from top leaf (leaf number 1)	leaf
cane_fraction	Fraction of accumulated biomass partitioned to cane	$g\ g^{-1}$
sucrose_fraction_stalk	Fraction accumulated biomass partitioned to sucrose	$g\ g^{-1}$
stress_factor_stalk	Stress factor for sucrose accumulation	nil
sucrose_delay	Sucrose accumulation delay	$g\ m^{-2}$
min_sstem_sucrose	Minimum stem biomass before partitioning to sucrose commences	$g\ m^{-2}$
min_sstem_sucrose_redn	Reduction to minimum stem sucrose under stress	$g\ m^{-2}$
tt_emerg_to_begcane	Thermal time required from emergence to start stalk growth	°C d
tt_begcane_to_flowering	Thermal time required from start of stalk growth to start of flowering	°C d
tt_flowering_to_crop_end	Thermal time from flowering to crop death	°C d
green_leaf_no	Green leaf number	leaves
tillerf_leaf_size	Expansion factor applied to leaf size due to tillering	nil
tillerf_leaf_size_no	Leaf number from top leaf (leaf number 1)	leaf

Table 1.2. DSSAT-Canegro cultivar parameters: Parameters represent morphological traits, developmental stages or physiological traits. Some parameters perform similar functions to APSIM-Sugar parameters such as leaf size and leaf number (*MXLFAREA* and *MXLFARNO*). Other parameters such as radiation use efficiency (*PARCEMAX* in DSSAT-Canegro; RUE in APSIM-Sugar) are variety specific in DSSAT-Canegro but are species specific in APSIM-Sugar.

Parameter	Description	Units
PARCEMAX	Maximum (no stress) radiation conversion efficiency expressed as assimilate produced before respiration, per unit of PAR	g MJ^{-1}
APFMX	Maximum fraction of dry mass increments that can be allocated to aerial dry mass	t t^{-1}
PCB	Partitioning coefficient: extinction coefficient of fraction of dry mass increments allocated to above-ground biomass	N/A
STKPFMAX	Fraction of daily aerial dry mass increments partitioned to stalk at high temperatures in a mature crop	t t^{-1}
DELTTMAX	Max. change in sucrose content per unit change in stalk mass in the unripened section of the stalk	t^{-1}
SUCA	Maximum sucrose contents in the base of stalk	t t^{-1}
TBFT	Temperature at which partitioning of unstressed stalk mass increments to sucrose is 50% of the maximum value	°C
Tthalfo	Thermal time to half canopy	°C d
Tbase	Base temperature for canopy development	°C
LFMAX	Maximum number of green leaves a healthy, adequately-watered plant will have after it is old enough to lose some leaves	leaves
MXLFAREA	Maximum leaf area assigned to all leaves above leaf number MXLFARNO	cm^2
MXLFARNO	Leaf number above which leaf area is limited to MXLFAREA	leaf
PI1	Phyllocron interval 1 for leaf numbers below Pswitch	°C d
PI2	Phyllocron interval 2 for leaf numbers above Pswitch	°C d
PSWITCH	Leaf number at which the phyllocron changes.	leaf
MAX_POP	Maximum tiller population	Stalks m^{-2}
POPTT16	Stalk population at/after 1600 degree days	Stalks m^{-2}
TTPLNTEM	Thermal time to emergence for a plant crop	°C d
TTRATNEM	Thermal time to emergence for a ratoon crop	°C d
CHUPIBASE	Thermal time from emergence to start of stalk growth	°C d
TT_POPGROWTH	Thermal time to peak tiller population	°C d
Lg_AMBASE	Aerial mass (fresh mass of stalks, leaves, and moisture) at which lodging starts	t ha^{-1}

Two important differences between APSIM-Sugar and DSSAT-Canegro are the approach to evapotranspiration (Singles, 2013) and the approach to biomass accumulation from photosynthesis (Lisson et al., 2005; Singles, 2013). APSIM-Sugarcane models transpiration using a transpiration efficiency approach whereby transpiration demand is a function of daily crop growth rate and transpiration use efficiency (Keating et al., 1999). DSSAT-Canegro calculates crop water requirements following the United Nations Food and Agriculture Organisations (FAOs) 'FAO 56' guidelines (Singels et al. 2008; Singels, 2013). APSIM-Sugar uses a radiation use conversion approach based on a linear relationship between radiation use efficiency and biomass produced while DSSAT-Canegro uses a more complex approach by simulating photosynthesis and respiration (Singles, 2013). The resulting difference in variety parameters exemplifies the need to carefully consider the influence of parameters on model outputs.

Above ground biomass accumulation in APSIM-Sugar is driven by a radiation use efficiency (RUE) approach where radiation refers to the 300 nm to 3000 nm bandwidth while DSSAT-Canegro simulates above and below ground biomass accumulation using a temperature dependent photosynthetically active radiation (PAR, 400 nm to 700 nm) conversion efficiency. Accumulated biomass in DSSAT-Canegro is then reduced by growth respiration (Singels, 2013). In DSSAT-Canegro this results in a variety specific radiation use parameter (*PARCEMAX*). APSIM-Sugar uses a calibrated RUE value of 1.8 g MJ^{-1} for plant crops and 1.65 g MJ^{-1} for ratoon crops. These values were derived from field experiments (Keating et al., 1999). Variability in RUE values reported in literature was considered to be a result of differences in trash recovery but RUE for sugarcane was assumed not to exceed 2 g MJ^{-1} (Robertson et al., 1996a; Sinclair and Muchow, 1999). In calibrating DSSAT-Canegro for two Brazilian sugarcane varieties Marin et al. (2011) increased *PARCEMAX* from 9.9 g MJ^{-1} (default value for South African variety NCO376) to 14.86 g MJ^{-1} for varieties RB72-454 and SP83-2847. Marin et al. (2014) suggested that this variety specific approach is more representative of observed variability in photosynthesis. The *PARCEMAX* parameter in DSSAT-Canegro and RUE in APSIM-Sugar are not directly comparable because of the differences in the biomass accumulation processes. However even a similar relative 50% increase of RUE in APSIM-Sugar would exceed observed limits (2.7 g MJ^{-1} compared to 2 g MJ^{-1}) and could greatly affect simulated yields. Clearly it is necessary for crop modellers to identify how changes in parameter values affect model outputs before calibrating models for specific varieties. Sensitivity analyses allows modellers to do this and are regularly employed as part of statistical model calibrations.

1.3. Sensitivity Analysis

Sensitivity analysis can be used to identify the model parameters that strongly affect simulated outputs (Makowski et al., 2006b; Monod et al., 2006). A sensitivity analysis can help in model calibration by identifying influential and uninfluential parameters. Parameters that are both influential and do not have a well validated value are ideal candidates for calibration. Sensitivity analysis techniques are largely defined as local or global (Saltelli et al., 2008). Local sensitivity analysis consider a small change in a single parameter value at a time while global sensitivity analysis considers how parameters affect the model over the whole range of parameter values. Global sensitivity analysis also considers parameter interactions (Saltelli et al., 1999). Saltelli and Annoni (2010) highlight the advantage of using global sensitivity analysis techniques for model assessment rather than the more traditionally used local and one-at-a-time (OAT; where a single parameter is considered) techniques. Pathak et al. (2007) used both local and global analysis for the CROPGRO-Cotton model, concluding that the global sensitivity analysis was an improvement over the local sensitivity analysis used.

1.3.1. Methods of global sensitivity analysis applied to crop models

Sensitivity analysis of crop models have used OAT methods such as the Morris method (Morris, 1991), regression methods such as Latin hypercube sampling and quasi-random LpTau (Confalonieri et al., 2010) and variance based methods such as the Sobol' method (Sobol, 1993), Fourier amplitude sensitivity test (FAST) (Cukier et al., 1973; Cukier et al., 1975; Schaibly and Shuler, 1973) and Extended-FAST (Saltelli et al., 1999) methods. The Morris approach was used to identify influential parameters for the STAMINA-Wheat model (Richter et al., 2010). The Extended-FAST method has been applied to various wheat models (Makowski et al., 2006b; Zhao et al., 2014; Jiang et al., 2011) as well as models for rice (Confalonieri, 2010; Confalonieri et al., 2010; Vanuytrecht et al., 2014) and maize (Dzotsi et al., 2013; Vanuytrecht et al., 2014).

Confalonieri et al. (2010) compared the application of Morris, regression and variance based methods to the Water Accounting Rice Model (WARM; Confalonieri et al., 2009) and detailed the different sensitivity measures used in each approach. The key advantage of the variance based methods is the ability to calculate first order or main effect indices (S_i) that measure the influence of a single parameter similar to OAT approaches, as well as joint effect indices (S_{ij}) that measure the influence of interactions between two or more parameters and the total effect index (ST_i) that measure the main effect as well as contributions from any interactions. An advantage of this is the ability to identify the influence of interactions. For example, by comparing S_i and ST_i, Zhao et al. (2014) concluded that variety parameter influence on wheat yields in APSIM-Wheat (Wang et al., 2003) were non-linear. This could have implications for the calibration of the APSIM-Wheat model. Wheat yields were largely influenced by three variety parameters (*grains.per.gram.stem*, *max.grain.size* and *potential.grain.filling.rate*) however, as these parameters were most influential through interactions, calibrating only these parameters would not be ideal. Further analysis of joint effects could identify what interactions are most influential and help identify which other variety parameters would need to be calibrated.

1.3.2. Efficiencies of global sensitivity analysis

Despite the evident advantages of variance based sensitivity analysis over OAT methods many modellers prefer OAT sensitivity analysis (Saltelli and Annoni, 2010). One advantage of OAT is the lower number of model runs needed. This is particularly relevant to crop models which can be computationally expensive. Confalonieri et al. (2010) concluded that the Morris method achieved similar rankings of parameter influence as the more computationally expensive Sobol and Extended-FAST method. The Extended-FAST and FAST methods are more efficient than the Sobol method (Saltelli et al., 2008). To improve the efficiency of variance based measures such as the Extended-FAST, several analyses have used the Morris method to screen for influential parameters on which to use the more rigorous variance based methods (Vanuytrecht et al., 2014; Zhan et al., 2013; Confalonieri, 2010). Reducing the number of parameters considered reduces the number of model runs that need to be performed. Removing the parameters from the more detailed analysis would preclude some potentially important interactions. An alternative method available is to calculate sensitivity indices from a model emulator or meta-model.

A model emulator or meta-model is a statistically simplified approximation of a more complex model (O’Hagan, 2006). If the simplified model is a close approximation of the actual model, sensitivity analysis can be performed on the computationally less expensive simplified model (Uusitalo et al., 2015). Uncertainty in the sensitivity of the emulator and the response of the actual model should be quantified as part of the emulation process (O’Hagan, 2006; Uusitalo et al., 2015). Statistical emulators have been built for the APSIM-Plant model (Ramankutty et al., 2013) and for sensitivity analysis of maize yield to weather conditions in the WOFOST model (Ceglar and Kajfež-Bogataj, 2012). However sensitivity analysis using model emulation is much more widely used in agent-based ecosystem models. For example a Bayesian approach to sensitivity analysis using a Gaussian emulator (Kennedy et al., 2006; Kennedy and O'Hagan, 2001) has been used for sensitivity analysis of land surface models (Petropoulos et al., 2014; Petropoulos et al., 2013) and a bird population model (Parry et al., 2013). Several other emulators have also been developed (Ratto et al., 2012).

1.3.3. Sensitivity analysis of sugarcane models

As part of a statistical calibration of the DSSAT-Canegro model Marin et al. (2011) conducted a sensitivity analysis to identify influential variety parameters. The sensitivity analysis was used to reduce the number of parameters that needed to be calibrated. The details of this sensitivity analysis were not published and no dedicated sensitivity analysis is available as part of documentation for either APSIM-Sugar or DSSAT-Canegro. From literature on the use of sensitivity analysis for crop and other complex models it is evident that greater insight into the effects of model parameters would greatly benefit sugarcane modelling research. Identifying influential parameters and parameter interactions could greatly streamline the calibration of variety parameters.

1.4. Statistical Calibration of Sugarcane Variety Parameters

Crop model parameters which are genotypic (variety specific) in nature must be identified and parameter values for each variety must be estimated to effectively simulate varietal differences (Jeuffroy et al., 2012). Zhou et al. (2003) suggested that parameter values should be stable across environments, vary significantly between varieties and be physiologically meaningful. Unfortunately due to the difficulty of obtaining data for specific varieties under specific conditions parameter values are often calibrated on data from a range of field experiments. Field experiments can be designed to provide the trait data required by crop models for new varieties so that multiple studies are not used in parameter estimation (Craufurd et al., 2013). However, running a new trial for all current varieties would not be cost efficient or feasibly practical. Statistical parameter estimation offers an alternative to conducting multiple field trials by making use of field trial data that already exists.

1.4.1. Types of statistical parameter estimation

Several studies have investigated the range of parameter estimation techniques that can be applied to crop models (Makowski et al., 2006a; Makowski and Wallach, 2002; Makowski et al., 2002; Tremblay and Wallach, 2004; Wallach et al., 2011). Parameter estimation techniques seek to optimise some type of 'goodness-of-fit' criterion between observed and simulated data (Wallach et al., 2011). For example, two standard nonlinear regression methods that can be used for parameter estimation are least squares regression and maximum likelihood regression

(Makowski et al., 2006a). The method of least squares uses the sum of squared differences between simulated and observed values as its goodness-of-fit measure and attempts to minimize this measure. Maximum likelihood regression uses a likelihood function as its measure of goodness-of-fit. The likelihood value is a measure of the probability that observed values would occur given a set of parameter values. Maximum likelihood regression seeks the estimated parameter set that maximises the likelihood value. Restricted maximum likelihood estimation was recently used to estimate parameter values for a customised wheat model for APSIM (Zheng et al., 2013). The complexity of crop models and a desire to better quantify the uncertainty in parameter estimations has led to an increasing use of genetic algorithms (Mitchell, 1999) as well as Bayesian (Gelman et al., 1997) parameter estimation techniques such as Generalised Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992) and Markov Chain Monte Carlo (MCMC) estimation (Geyer, 1992).

1.4.1.1. Genetic algorithms

Genetic algorithms are based on the ideas of evolution and natural selection. There are many forms of genetic algorithms of varying complexity. All genetic algorithms follow a structure similar to a generic breeding program in which hypothetical ‘parent’ varieties are simulated and allowed to cross to produce new varieties. Crosses between parents are based on a goodness-of-fit criterion so that parent varieties that better represent the given data are more likely to be used in the next generation of parameter estimates. Genetic algorithms provide robust solutions, have good global conversion and allow the researcher to investigate the parameter space more fully than regression approaches (He et al., 2012). Although genetic algorithms excel at general solutions, the process is computer intensive and may not converge to a precise solution (Voit, 2013). Genetic algorithms have been used to parameterise generic crop models (Bulatewicz et al., 2009; Klein et al., 2012) as well as models designed for specific crops (Dai et al., 2009; He et al., 2012) but have not found application in sugarcane crop models.

1.4.1.2. Bayesian statistics

Bayes’ rule provides a method to update our belief in the probability of a model systematically as more data becomes available. Specifically Bayes’ rule states that the posterior probability of a model given some new observations ($P(model \mid observation)$) is proportional to the product of the prior probability of the model ($P(model)$) and the probability of the new observations occurring under that model ($P(observation \mid model)$; known as the likelihood): $P(model \mid observation) \propto (P(model)) \times P(observation \mid model)$. The advantage of using Bayesian statistics is that parameter estimation takes into account prior knowledge of the nature of parameter values to describe a posterior probability based on observations. This allows researchers to estimate parameters from different data sources and perform uncertainty analysis (Makowski et al., 2006a).

The reporting and handling of model uncertainty has become a major concern as the use of climate change and process-based crop models has increased (Angulo et al., 2013; Challinor et al., 2013; Hawkins et al., 2013; Lobell, 2013). Kennedy and O'Hagan (2001) identified six types of uncertainty in model outputs: parameter uncertainty, model inadequacy, residual variability, parametric variability, observation error and code uncertainty. Kennedy and O'Hagan (2001) propose a novel Bayesian approach to model calibration that can better capture these sources of output uncertainty. Unfortunately this method has not been applied to crop models in the available literature. Two Bayesian approaches that have found application in crop models are the Markov Chain Monte Carlo (MCMC) estimation and Generalised Likelihood Uncertainty Estimation (GLUE).

The MCMC approach simulates a random walk that converges on the posterior probability distribution ($P(model \mid observation)$). MCMC is an iterative process that requires an initial parameter estimate and prior (proposal) distribution. Several starting parameter estimates can be used in order to better cover the available parameter space. The MCMC process can be outlined as:

1. Select a starting model as a set of parameter values from the prior distribution;
2. Generate a random (candidate) parameter set based on a sampling distribution;
3. Calculate an acceptance criteria based on the ratio of the posterior probabilities for the initial and candidate parameter sets such as the Metropolis algorithm (Metropolis et al., 1953) or Metropolis-Hastings algorithm (Hastings, 1970);
4. If the acceptance criteria is greater than a number randomly selected from a uniform distribution between 0 and 1, then the candidate parameter set is accepted as the new model, otherwise repeat steps 2-3
5. Steps 2 to 4 are repeated to form a chain until all parameters reach approximate convergence (Gelman et al. 1997).

MCMC algorithms have been used to parameterise crop models for rice (Iizumi et al., 2011; Iizumi et al., 2009), maize (Tao et al., 2009) and wheat (Tao and Zhang, 2013; Dumont et al., 2014) as well as the generic Plant module in APSIM (Archontoulis et al., 2014) but have not been applied to sugarcane crop models.

In contrast to MCMC simulations, GLUE does not generally require an iterative process. A simplistic overview can be outlined in four steps

1. A prior probability distribution is developed for each parameter;
2. A Monte Carlo approach is used to generate a large number (*N*) of random samples of parameter sets from the prior distribution;
3. Calculate likelihood for each parameter set using an appropriate likelihood function;
4. Construct a posterior probability distribution for each parameter.

While GLUE was developed with the assumption that the choice of likelihood function was ambiguous (Beven and Binley, 1992) the choice can affect the accuracy of the estimated posterior distribution (He et al., 2010). GLUE has been used effectively for parameterising generic crop models (Wang et al., 2005) as well as crop models for maize (He et al., 2010), wheat (Mo and Beven, 2004), cotton (Pathak et al., 2012) and variety parameters for sugarcane in DSSAT-Canegro (Marin et al., 2011). DSSAT V4.5 comes pre-installed with a GLUE utility to estimate variety parameter values for any crop within the DSSAT system (Jones et al., 2011).

1.4.2. Statistical calibration for sugarcane crop models

The use of MCMC and GLUE in crop modelling research suggests that these techniques should be explored for application to sugarcane crop models. Marin et al. (2011) estimated variety parameters for two Brazilian sugarcane varieties using GLUE. Model predictive capability in Marin et al. (2011) was expressed as the normalized distance measure: 'modelling efficiency' (Eff) using leave-one-out cross validation (Wallach, 2006). The measure Eff ranges from $-\infty$ to 1. A model with an Eff of 1 exactly replicates observed data. A model with an Eff of 0 would have the same agreement as using the average observed value for every observation and is generally considered a poor model. A negative Eff value would suggest the model performed worse than using the average observed value to predict every observation. Across all observations of both varieties, cross-validated modelling efficiency (Eff_{CV}) was good for aerial dry biomass ($Eff_{CV} = 0.85$) and stalk dry mass ($Eff_{CV} = 0.765$) but relatively poor for sucrose ($Eff_{CV} = 0.170$) and number of green leaves ($Eff_{CV} = -2.300$). The two varieties were also assessed individually but no attempt was made to directly compare the calibration of the two varieties (i.e. whether differences in estimated parameter values were realistic). To truly assess whether GLUE or any statistical calibration is appropriate for use with sugarcane models more research is needed to assess if calibrated parameter values are accurate rather than comparisons of observed and simulated yields.

Makowski et al. (2002) compared MCMC and GLUE approaches applied to a linear-plus-plateau model similar to a model of crop yield response to applied nitrogen. The 22 parameters of the model and model output error were pre-defined to perform a theoretical comparison. In this way Makowski et al. (2002) were able to assess MCMC and GLUE performance based on mean squared error of prediction (MSEP) of model outputs (observed data vs model outputs) as well as comparing estimated parameter values to pre-defined values. The authors concluded that both MCMC and GLUE produced accurate results based on MSEP of output but recommend MCMC. Although Makowski et al. (2002) did not directly compare estimates of parameter values it was possible to identify that in that study MCMC was able to estimate 9 of 22 parameters to within 10% of their true values while GLUE was able to estimate 7 of 22 parameters to within 10%. A theoretical comparison such as that performed by Makowski et al. (2002), should be considered to help evaluate the appropriateness of statistical parameter estimation techniques for sugarcane crop models.

1.5. Conclusion

Sugarcane is an important agronomic crop globally and sugarcane industries world-wide continuously strive to improve crop productivity. This has been accomplished by improving farm management practices as well as by breeding sugarcane varieties for improved yields, resistance to pests and diseases as well as resistance to abiotic stresses such as water stress. While sugarcane crop models have been used to help improve management practices such as irrigation and fertilizer application or timing of harvest, little research has been conducted in simulating differences in traits between varieties. Crop models have been used in a range of other agronomic crop industries to investigate interactions between varieties, environments and management. This has been achieved by modifying variety parameters that represent different physiological traits. Before sugarcane modelling can truly advance in this field a better understanding of the strengths and limitations of sugarcane crop models in simulating varietal differences is needed. Given the continuous development of sugarcane varieties crop modellers should also consider how well current models reflect growth of current commercial varieties.

One approach to better understand the impact of variety parameters in sugarcane crop models is to perform a statistical sensitivity analysis. A sensitivity analysis can identify how model outputs such as yield, are influenced by specific parameters in the model. Simulation experiments can be designed to consider how this influence changes under different environmental or management conditions. Given the complexity of sugarcane crop models, variance based sensitivity measures should be used to identify main effects and any possible parameter interactions. Due to the relatively large number of parameters defined in a crop model and computational expense, it would be worthwhile for sugarcane crop modellers to consider efficient sensitivity approaches such as the use of model emulators. A better understanding of the influence of variety parameters would benefit sugarcane crop modelling research by helping to streamline model calibration.

Internationally recognised crop models such as APSIM-Sugar and DSSAT-Canegro have played an important role as decision support tools for sugarcane. However, these sugarcane models have not yet reached the level of success in trait modelling developments that has been reached by crop models for crops such as grains or legumes. Statistical calibration techniques applied to models for grains and legumes may not have the same success applied to sugarcane models as grain and legume crops focus on determinate processes such as flowering while sugarcane relies on vegetative growth. While GLUE has been applied to the DSSAT-Canegro model (Marin et al., 2011) no formal comparison of calibration techniques has been performed to assess the accuracy of estimated parameter values. Future research should aim to assess the effectiveness of a range of techniques such as genetic algorithms, GLUE and MCMC.

Trait modelling will enable researchers to better investigate desirable traits and variety, environment and management interactions that affect current commercial varieties. In order to achieve effective modelling of varietal differences sugarcane modellers must:

1. Identify the current ability of sugarcane crop models to simulate varietal differences (Chapter 2);
2. Investigate the influence variety parameters have on key model outputs, using statistical sensitivity analysis (Chapter 3) and

3. Investigate whether statistical calibration techniques applied to other crop models are appropriate and effective for sugarcane models (Chapter 4).

Achieving these goals will make sugarcane models a better decision support tool for sugarcane industries.

1.6. Chapter 1 Summary

As one of the highest biomass producing crops in the world, sugarcane has the potential to contribute a solution to the demands of a growing global population. The sugarcane industry must continuously improve crop productivity to meet demands while remaining environmentally and economically sustainable. Improvements to sugarcane productivity have been made by breeding new varieties, improving farm technology and developing farm management strategies for specific environments. Further improvements to crop productivity are difficult to achieve due to the complex interactions between varieties, environments and management strategies. Crop models simulate productivity under a range of environments and management schemes allowing researchers to explore interactions without the expense of field experiments. Although sugarcane models have been widely used as decision support tools the effect of varietal differences has not been an area of focus in sugarcane research. In contrast, simulation of varietal traits has been used to study historical crop improvement, identify physiological traits that confer a yield advantage and investigate the trade-offs between yield and disease resistance for other crops such as wheat, soybeans and peaches. Clearly the sugarcane industry requires a better understanding of the capability of sugarcane models to simulate varietal differences. Chapter 1 considered how sugarcane models represent varietal differences and the statistical tools such as sensitivity analysis and calibration techniques that can be used to improve the relevance of sugarcane models. In order to achieve effective modelling of varietal differences sugarcane modellers must:

1. Identify the current ability of sugarcane crop models to simulate varietal differences (Chapter 2);
2. Investigate the influence variety parameters have on key model outputs using statistical sensitivity analysis (Chapter 3) and
3. evaluate the use of statistical calibration techniques applied to other crop models for variety parameters in sugarcane models (Chapter 4).

Achieving these goals will help improve sugarcane models as a decision support tools for the sugarcane industry.

Chapter 2

Detailed trait characterisation is needed for simulation of variety responses to water stress

Relevant publication	Sexton, J., Basnayake, J., Everingham, Y., Inman-Bamber, G., Lakshmanan, P., Jackson, P., 2014. Detailed trait characterisation is needed for simulation of cultivar responses to water stress, Proceedings of the Australian Society of Sugar Cane Technologists: Gold Coast, Queensland, Australia.
Statement of intellectual input from co-authors	The research question was developed with input from Sexton, Everingham and Inman-Bamber. Field trial data were supplied by Basnayake on behalf of the More Crop Per Drop project funded by the Sugar Research and Development Corporation as project BSS334. Jackson supplied pot trial data used to generate transpiration efficiency parameter range. Inman-Bamber provided template simulation files used to model the field trial data and provided assistance with interpreting simulation output. Sexton updated and modified these files to run the project simulations. Sexton wrote the original draft of the paper which was revised with input from Basnayake, Everingham, Inman-Bamber, Lakshmanan and Jackson. Sexton performed data analysis and produced all figures and tables.
Publication status	Published

2.1. Introduction

The Agricultural Production Systems sIMulator (APSIM; (Keating et al., 1999)) has been used in Australia as a decision support system. Applications for sugarcane have included irrigation scheduling (Everingham et al., 2008; Inman-Bamber et al., 2006), fertiliser management (Attard et al., 2008) and seasonal yield forecasts (Everingham et al., 2009). The adoption of decision support systems such as APSIM is difficult to achieve as end users require a specific skill set to interpret the model outputs. The difficulties of achieving adoption of such 'knowledge intensive' decision support systems have been investigated for a range of agricultural industries in Australia (Hayman, 2004; Hochman et al., 1994; Hochman and Carberry, 2011; McCown et al. 2002) including within the Australian sugarcane industry (Everingham et al., 2006; Jakku et al., 2007; Thorburn et al., 2011). Everingham et al. (2006) reported on the need for collaborative workshops between growers, extension officers and researchers for end users to gain confidence in modelling in the areas of fertiliser management, irrigation scheduling and climate forecasts. The development and adoption of the irrigation model WaterSense (Inman-Bamber et al., 2007) within the Australian sugar industry provides an example of the benefits of such participatory research as a common learning experience for both end users and model developers.

Crop models have not yet been applied to assisting sugarcane breeding programs. However, it is hypothesised that accurately simulating differences between varieties will allow researchers to better identify and select varieties predicted to perform well in different environments (Jeuffroy et al., 2006). APSIM has been used to simulate genotype by environment interactions in sorghum under various environments (Chapman, 2008). Analysing variety traits through simulations or 'trait modelling' is also a developing area of research in a range of other commercial crop industries such as soybeans (Boote et al., 2001), peanuts (Putto et al., 2013) and peaches (Quilot et al., 2012).

Desktop studies using the 'Sugar' module (Keating et al., 1999) in APSIM (APSIM-Sugar) to date have placed minimal focus on variety effects. In fact in the application studies mentioned above (Attard et al., 2008; Everingham et al., 2009; Inman-Bamber et al., 2006) the variety used in simulations was not mentioned at all. The lack of detailed understanding of variety simulations restricts sugarcane researchers from exploring the potential advantages of variety specific simulation studies identified in other crop industries.

Research on developing sugarcane for water-limited environments has gained more momentum recently. However, the effects of water stress on sugarcane are complex. Previous research has identified some differences in varietal responses to water stress (Inman-Bamber and Smith, 2005; Lakshmanan and Robinson, 2013). More recently, Basnayake et al. (2012b) investigated commercial varieties and introgression clones (developing varieties) under irrigated and water stressed conditions. Basnayake et al. (2012b) identified a relatively low genotype by treatment interaction on cane and sugar yields for both commercial varieties and introgression clones under mild to moderate stress conditions but larger variety by treatment interactions under severe stress. Identifying physiological parameters that contribute most to the observed variety by water stress level interactions remains a major challenge.

Simulation studies are capable of investigating the impact of physiological traits on varietal performance without field trials. Inman-Bamber et al. (2012) identified increased intrinsic (leaf level) transpiration efficiency, increased rooting depth and reduced stomatal or root conductance as beneficial traits under water stressed conditions. These traits are difficult to characterise for different varieties and have not been calibrated for each variety in sugarcane crop models. For example the transpiration efficiency parameter (*transp_eff_cf*) in APSIM-Sugar is a constant value for all sugarcane varieties even though there is evidence to suggest transpiration efficiency varies across genotypes and environmental conditions (Basnayake et al., 2012a; Jackson et al., 2014).

Transpiration efficiency (TE) is defined as the ratio of biomass gained to total water used by the plant (transpiration) and is inversely proportional to vapour pressure deficit (VPD) (Inman-Bamber et al., 2012). In APSIM the intrinsic TE parameter (*transp_eff_cf*) is defined as the TE at a VPD of 1 kPa. Transpiration rates are calculated on a daily time step based on daily calculated VPD. Transpiration rates were not directly measured in the original build of APSIM-Sugar. Instead *transp_eff_cf* was obtained by calibration to datasets exhibiting water deficits and has been applied as a constant value of 0.008 g of biomass per g of water at a VPD of 1 kPa (Keating et al., 1999). As TE has been found to differ between varieties it is important for modellers to assess how modifying *transp_eff_cf* within APSIM-Sugar may affect important simulation outputs.

Sugarcane modelling research has the potential to expand into variety modelling research currently practiced by a range of other commercial crop industries. However, the current capacity of APSIM-Sugar to simulate varietal differences must first be determined. The objectives of this chapter were to investigate the current capability of APSIM-Sugar to simulate differences between varieties under irrigated and stressed conditions (Objective 1 of the Thesis) and to motivate the need for research into model sensitivity analysis (Objective 2 of the Thesis). The TE parameter in APSIM-Sugar is used as an example of the potential influence modifying parameter values can have on simulated yields. Transpiration efficiency was chosen as it has recently been shown to vary between varieties but is not considered a variety parameter in APSIM-Sugar. This chapter considers only physiological traits as APSIM-Sugar cannot accommodate traits such as pest and disease resistance.

2.2. Materials and Methods

2.2.1. Field trial data

Yield data for four commercially released sugarcane varieties were collected from a water stress research trial performed at Home Hill in Queensland, Australia. Basnayake et al. (2012b) fully documented the details of the Home Hill experiment. For ease of reference, planting and harvest dates for the Home Hill trials are reproduced in Table 2.1. A total of 89 clones were grown under fully irrigated and water stressed conditions for the plant and two ratoon crops at Home Hill (a total of 6 environments). Although they are no longer grown for commercial production, the present study focuses on varieties Q117, Q124, Q138 and R570 because these were the only varieties in the Home Hill experiment that have been described to some extent in APSIM-Sugar v7.5. The yield data consisted of biomass yields at harvest collected as above-ground total dry matter (Figure 2.1). Total dry matter was estimated from fresh and dry weights of a subsample of eight mature stalks. Samples were collected randomly from the two middle rows of each plot with two replicates per variety (Basnayake et al., 2012b). Pests and diseases were controlled by following commercial crop production practices.

Table 2.1. A summary of experimental conditions of the Home Hill field trial

Attributes	Details
Location	147°23’ E, 19°41’ S
Soil texture	Light Clay; Plant Available Water Capacity (PAWC) = 220.1mm based on simulation Daily Upper Limit and Lower Limit.
Planting date	17 June 2007
Harvest date	17 June 2008 (Plant) 15 June 2009 (1st Ratoon) 14 June 2010 (2nd Ratoon)
Experimental design	Split plot, water supply as whole plots and varieties as sub-plots, two replicates were recorded for each variety and treatment combination

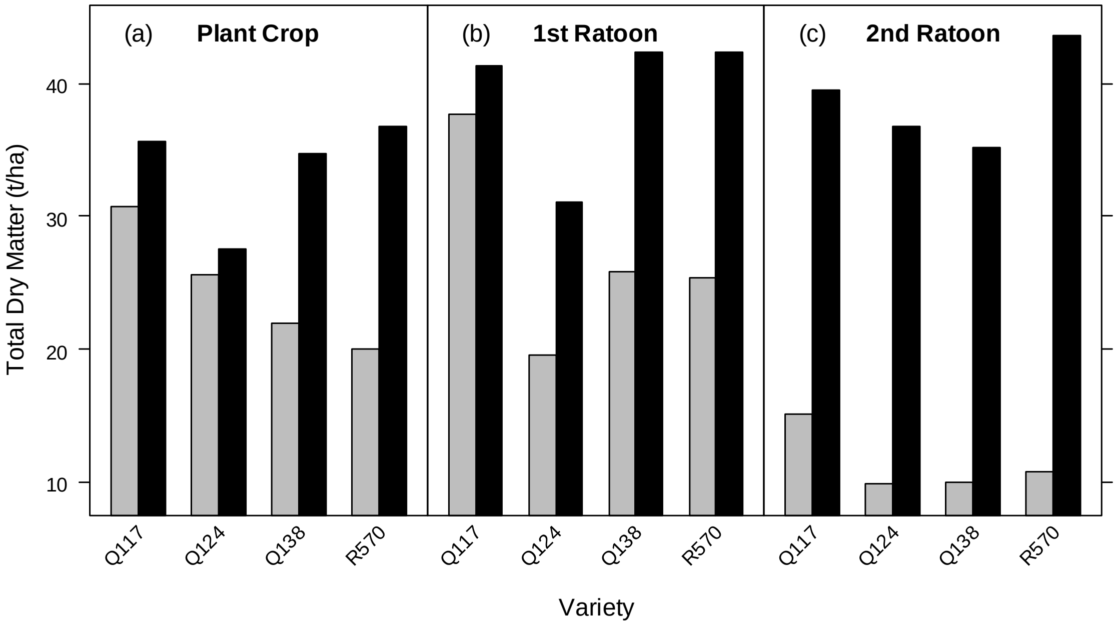

Figure 2.1. Mean observed total dry matter yields of two replicates for the (a) plant, (b) first ratoon and (c) second ratoon crops for water stressed (grey) and fully irrigated (black) treatments at Home Hill.

2.2.2. APSIM-Sugar model configuration

The latest version of APSIM-Sugar (v.7.5) was parameterised to represent field trial conditions following the work of Basnayake et al. (2012b). Hilling up and pesticide application were assumed to have no effect on yield in the simulations. Although herbicides were used to control weeds in all treatments, weed competition was observed in the plant crop and the effects of weed competition were included in the simulation by reducing the effective RUE prior to the stalk elongation stage by half (0.65 g MJ^{-1} from 1.8 g MJ^{-1}). The modification to RUE helped account for poor growth in the plant crop producing simulated above-ground biomass closer to observed measures of total dry matter. The adjustment for weeds in the plant crop was applied to all varieties. The TE parameter (*transp_eff_cf*) was modified from the default 0.008 g kPa g^{-1} to 0.0087 g kPa g^{-1} based on the work of (Inman-Bamber and McGlinchey, 2003) who reported the only field-based measure of TE in sugarcane. The effect of stress applied to expansive growth was also modified following Basnayake et al. (2012b). By default in APSIM-Sugar, the effect of soil water deficit on leaf expansion increases linearly from 0 to 1 from a soil water demand ratio of 0.1 to 0.6. This was modified so that the effect of soil water deficit on leaf expansion increased from 0 to 1 for a soil water demand ratio of 0.3 to 1.5. This was justified in Basnayake et al. (2012b) as "[The] default renders leaf expansion less responsive than photosynthesis to water stress which is not correct." (Basnayake et al. (2012b) supplementary data table S3).

For the irrigated treatment, lodging was simulated to occur, based on cane biomass and recent rainfall (Inman-Bamber et al., 2004). The effects of lodging were simulated by reducing effective RUE by 20% (Basnayake et al. 2012b; supplementary table S3). Lodging was simulated to occur in the plant crop (18th April 2008) and both the first (3rd February 2009) and second (14th January 2010) ratoons. Simulated lodging dates were considered realistic as lodging was noticed in the irrigated treatments after the eight-month period, although exact lodging dates were not recorded. Lodging was not simulated in the water stress treatment, however loss of stalk biomass due to water stress was. Stalk loss was simulated as a loss of 0.5 stalks/m^2/day if leaf area index (LAI) was reduced below 0.5 after having exceeded an LAI of 2 (Inman-Bamber et al., 2012). Stalk loss due to stress was simulated to occur during the second ratoon (26th December 2009) under water stress conditions.

2.2.3. Variety independent validation of APSIM-Sugar

Simulated above-ground biomass yields at harvest for variety Q117 were compared to the mean of all observed above-ground total dry matter for varieties Q117, Q124, Q138 and R570 combined. The standard error of the mean of the four varieties was also calculated. The simulated growth over time was analysed although only final harvest yields were available. Comparisons between simulated Q117 and the mean of the four varieties were made as observed data for individual varieties was low (only two replicates available). This prohibited a statistical analysis of the simulation so that only a descriptive analysis was performed. Comparisons were made to identify if the observed differences in yields between environments was captured in the simulations.

2.2.4. Simulation of varietal differences

Biomass yields (above-ground biomass) were then simulated using variety definitions in APSIM-Sugar for Q117, Q124, Q138 and R570 respectively (Table 2.2). Sugarcane varieties within the current version of APSIM-Sugar (v7.5) vary with respect to leaf size *(leaf_size, leaf_size_no, tillerf_leaf_size, tillerf_leaf_size_no*), biomass partioning (*cane_fraction, sucrose_fraction_stalk, sucrose_delay, min_sstem_sucrose, min_sstem_sucrose_redn*) and the thermal time required from emergence to cane development (*tt_emerg_to_begcane*) (Inman-Bamber and McGlinchey, 2003; Keating et al., 1999). Varieties Q117 and Q124 differ only in tiller leaf size while variety Q138 also differs with respect to accumulation of sucrose. Variety R570 has a high leaf area compared to several other varieties (Inman-Bamber, 2013; Cheeroo-Nayamuth et al., 2000), which is reflected in APSIM-Sugar. Comparisons between simulated biomass yields (above-ground biomass) and observed yields (above-ground total dry matter) were explored descriptively for each variety in each environment.

Table 2.2. Variety parameters in APSIM-Sugar and their values for Q117, Q124, Q138 and R570.

Parameter	Units	Q117	Q124	Q138	R570
leaf_size (*leaf_size_no*)	mm^{2}	1500(1)	1500(1)	1500(1)	3000(1)
		55000(14)	55000(14)	55000(14)	7000(4)
		55000(20)	55000(20)	55000(20)	10000(6)
					45000(10)
					60000(14)
					60000(20)
cane_fraction	leaf	0.70	0.70	0.70	0.68
sucrose_fraction_stalk	g g^{-1}	1.0(0.2)	1.0(0.2)	1.0(0.2)	1.0(0.2)
(*stress_factor_stalk*)		0.55(1.0)	0.55(1.0)	0.61(1.0)	0.58(1.0)
sucrose_delay	g g^{-1}	0	0	600	0
min_sstem_sucrose	g	800	800	1500	693
min_sstem_sucrose_redn	g	10	10	10	10
tt_emerg_to_begcane	g	1900	1900	1900	1500
tt_begcane_to_flowering	g	6000	6000	6000	6000
tt_flowering_to_crop_end	°C d	2000	2000	2000	2000
green_leaf_no	°C d	13.0	13.0	13.0	13.0
tillerf_leaf_size	mm^{2} mm^{-2}	1(1)	1(1)	1(1)	6(1)
(*tillerf_leaf_size_no*)		1.5(6)	1(4)	1(4)	1(12)
		1.5(10)	1.5(10)	1.5(10)	
		1(12)	1(16)	1(16)	
		1(26)	1(26)	1(26)	

2.2.5. Sensitivity of simulated biomass to TE

Each variety was then simulated using a range of plausible values for the TE parameter (*transp_eff_cf*). Values from 0.005 g kPa g^{-1} to 0.014 g kPa g^{-1} at an increment of 0.0001 g kPa g^{-1} were used to simulate each variety for the 1st ratoon. By simulating biomass yield (above-ground biomass) for a range of *transp_eff_cf* values it was possible to explore the effect that different levels of TE had on simulations of biomass yields for the irrigated and water stressed simulations (i.e. the sensitivity of simulated biomass yields to changes in *transp_eff_cf*. It was also possible to identify what values of the *transp_eff_cf* resulted in simulated biomass yields (above-ground biomass) close to observed biomass yields (above-ground total dry matter) assuming differences in *transp_eff_cf* values between varieties could explain all observed differences in biomass yields.

Standard regression analysis statistics such as the coefficient of determination (r^2) were inappropriate for analysis of the current data set due to the low availability of independent observed data. Comparisons between simulations and observed data and the effects of varying *transp_eff_cf* were analysed descriptively.

2.3. Results and Discussion

2.3.1. Variety independent validation of APSIM-Sugar

Simulated final yields for variety Q117 closely followed the mean observed yield of the four varieties (Q117, Q124, Q138 and R570) for each crop under both water stressed and irrigated treatments (Figure 2.2). Simulated yields were within one standard error of the observed mean of the four varieties for all six environments. The simulation of differences between environments was considered accurate enough to investigate simulations of relative varietal differences.

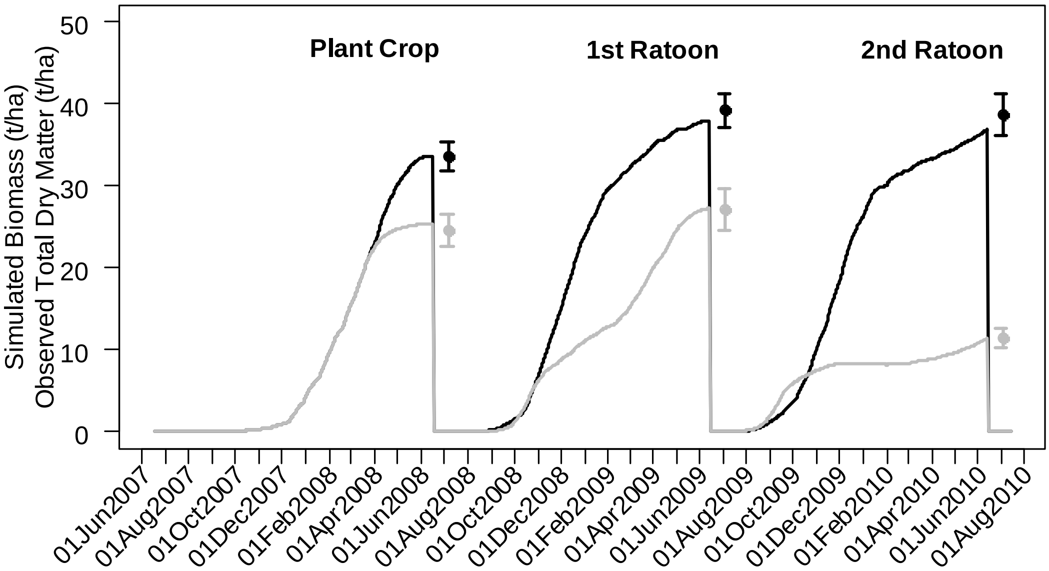

Figure 2.2. Simulated biomass yield (above-ground biomass) for Q117 for water stress (—) and irrigated (—) treatments over time. Solid points represent the mean observed biomass yield (as above-ground total dry matter) across all varieties (Q117, Q124, Q138 and R570) for water stress and irrigated treatments at Home Hill, for the plant, first ratoon and second ratoon crops. Vertical ‘whiskers’ identify +/- 1 standard error from the mean of all varieties. Simulations assumed a constant *transp_eff_cf* of 0.0087 g kPa g^{-1} for all varieties.

2.3.2. Simulation of varietal differences

Figure 2.3 displays variations in observed biomass yields (above-ground total dry matter) and simulated biomass yields (above-ground biomass) among varieties in the field trial. Observed differences between varieties varied between crops and treatments. Under irrigated conditions Q124 had a lower mean yield than any other variety in the plant and 1st ratoon crops while Q117 and Q138 had similar mean observed yields. For the 2nd ratoon crop Q138 had the lowest observed mean yield. Variety R570 had slightly higher mean observed yields than other varieties for the plant and 2nd ratoon crops under irrigated conditions.

Under stressed conditions variety Q117 had the highest observed mean yields for each crop. Between variety differences in observed yields varied for each crop under stressed conditions. For the 1st ratoon differences between observed variety yields were similar for stressed and irrigated treatments. However for the plant and 2nd ratoon the differences between varieties varied between irrigated and stressed treatments.

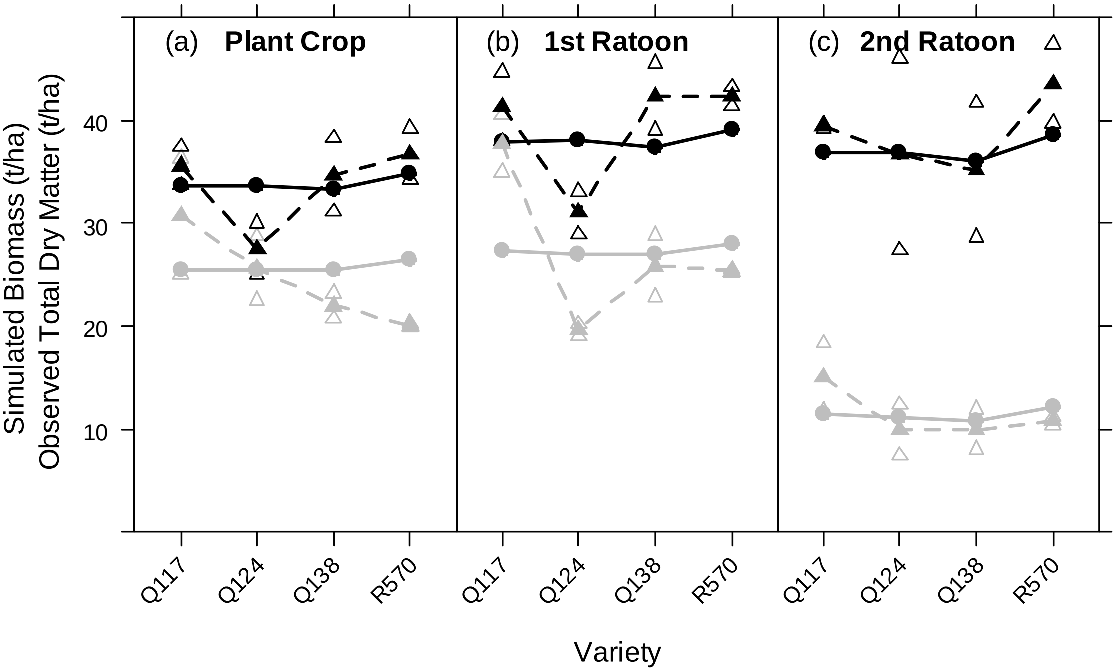

Figure 2.3. Comparison of observed biomass yields (above-ground total dry matter) and variety specific simulated biomass (above-ground biomass) for the (a) plant (b) first ratoon and (c) second ratoon crops. Open triangles represent observed replicates for water stress (△) and irrigated (△) treatments and closed triangles represent the observed mean (–▲–, –▲–). Closed circles represent the simulated biomass yields under water stressed (-●-) and irrigated (-●-) treatments. Simulations assumed a constant *transp_eff_cf* of 0.0087 g kPa g^{-1} for all varieties.

In comparison to observed yields, simulated yields for different varieties appeared very similar under all environments (Figure 2.3). There was virtually no simulated difference between varieties Q117, Q124 and Q138 across all environments while R570 consistently had the highest simulated yield. Simulations for Q117, Q124 and Q138 were identical for the plant crop water stress treatment while Q117 and Q124 were identical for the irrigated treatment. In the 2nd ratoon under stressed conditions there was less observed variability between varieties and the simulations of Q124, Q138 and R570 closely align with the mean observed yields. However, simulations did not capture the three most evident observed differences between varieties; the lower yield of Q124 under irrigated conditions of the plant and 1st ratoon, the higher yield of Q117 under stressed conditions and how differences between varieties changed under stressed conditions most evident in the plant and 2nd ratoon.

The lack of any difference between simulations for Q117, Q124 and Q138 was caused by the almost identical description of these varieties in APSIM-Sugar (Table 2.2). Parameters within APSIM-Sugar for one or more of these varieties may be inaccurate. While all three varieties were simulated identically, Bonnett (1998) calculated significantly different leaf appearance rates between varieties Q117 and Q138. It is possible therefore that these varieties differ at least in leaf characteristics. R570 is characterised quite differently within APSIM-Sugar. This may have contributed to the more accurate simulation of the difference between R570 and Q varieties under irrigated conditions for the plant and 2nd ratoon crops. However, as with the Q varieties response to water stress was not captured. The results of this study agree with the opinion of O'Leary (2000) that crop model improvement is required to improve the simulation of sugarcane responses to stress.

2.3.3. Sensitivity of simulated biomass to TE

Incrementing *transp_eff_cf* in APSIM-Sugar had a large effect on simulated biomass yields (above-ground biomass) (Figure 2.4). The response of simulated biomass yields to changes in *transp_eff_cf* values differed between the simulations of irrigated and stressed treatments. Under stressed treatments final yield increased linearly with an increase in *transp_eff_cf* for the 1st ratoon. An increase in *transp_eff_cf* also linearly increased simulated yields under irrigated conditions before a plateau was reached. As *transp_eff_cf* is increased in APSIM-Sugar, less water is required for a crop of the same size, resulting in less simulated stress and therefore higher yields can be achieved. This explains the increase in yield with an increase in *transp_eff_cf*. When water stress is not present biomass is limited by other stresses (such as nutrient stress) or by RUE and an increase in TE (*transp_eff_cf*) will not increase yields. This explains the plateau in simulated biomass yields under irrigated conditions. High values of *transp_eff_cf* resulted in larger simulated biomass yields for the simulation of the water stressed treatment than for the simulation of the irrigated treatment. This was likely a result of different levels of RUE between the two treatments. Lodging was simulated to occur in the irrigated treatment for the first ratoon but was not included in the simulation of the stressed treatment. As the effects of lodging were simulated by reducing RUE, the maximum unstressed biomass that could be simulated was lower for the simulation of the irrigated treatment than for the simulation of the water stressed treatment. A similar effect was documented in a field experiment, where lodging in a high irrigation treatment significantly reduced total biomass, cane yields and sucrose yields compared to lower levels of irrigation (Inman-Bamber et al. 2004).

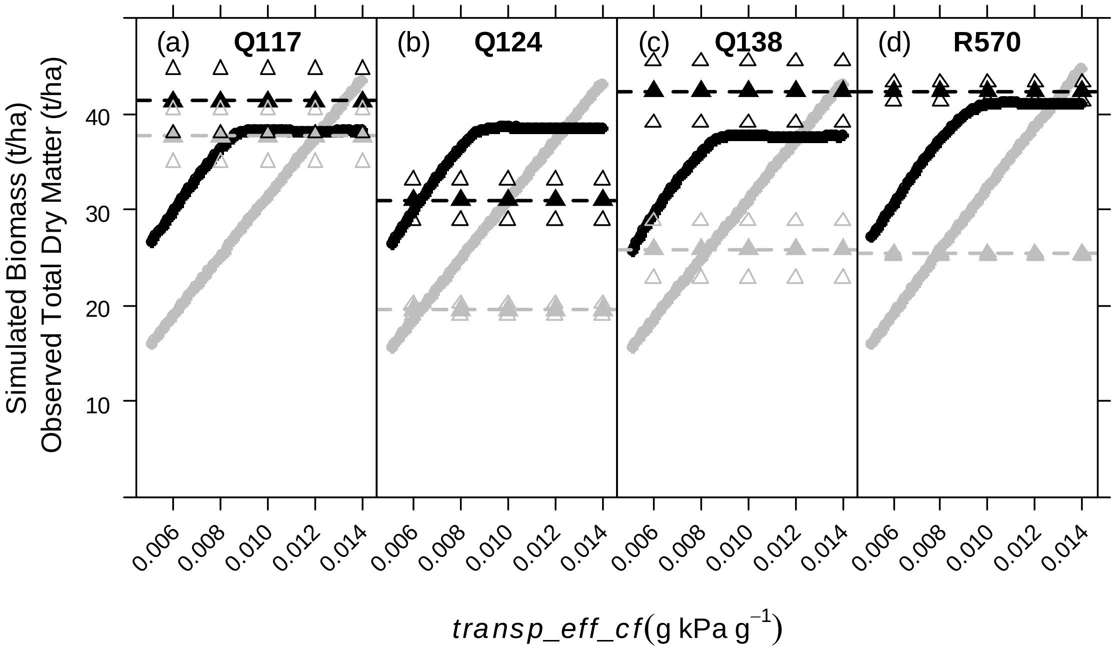

Figure 2.4. Comparison of observed biomass yields (above-ground total dry matter) and simulated biomass yields (above-ground biomass) using a range of *transp_eff_cf* values for variety (a) Q117, (b) Q124, (c) Q138 and (d) R570. Open triangles represent observed yield replicates for water stress (△) and irrigated (△) treatments and closed triangles represent the observed mean (–▲–, –▲–). Closed circles represent the simulated biomass yields under water stressed (-●-) and irrigated (-●-) treatments.

Simulated biomass yields (above-ground biomass) for each variety were closest to mean observed biomass yields (above-ground total dry matter) for different *transp_eff_cf* values in the first ratoon crop, most notably for the stressed treatment (Figure 2.4). For the stressed treatment the simulated biomass yield of Q117 was closest to the mean observed biomass yield for a *transp_eff_cf* value of 0.0121 g kPa g^{-1} while for Q124 simulated yield was closest to mean observed yield for a *transp_eff_cf* value of 0.0064 g kPa g^{-1}. Simulated yields for Q138 and R570 were closest to mean observed yields for *transp_eff_cf* values of 0.0083 g kPa g^{-1} and 0.0078 g kPa g^{-1} respectively under stressed conditions. These 'calibrated' values of *transp_eff_cf* for Q117 and Q124 differ considerably from the default value of APSIM-Sugar (0.0080 g kPa g^{-1}) and the measured value for Q127 (0.0087 g kPa g^{-1}) reported by Inman-Bamber and McGlinchey (2003). There were also obvious differences between *transp_eff_cf* values for stressed and irrigated treatments for each variety. However, these results must be interpreted very carefully.

There was a relatively high variability in observed yield replicates for Q117 and Q138 under stressed conditions (Figure 2.4) and further variability would arise if plant and ratoon crops were included. Directly comparing simulated results for various *transp_eff_cf* values with observed results assumes that all variability between varieties could be explained by differences in TE. Obviously any single parameter could be 'tuned' in this way to force simulated data to match observations. Furthermore higher simulated biomass yields under stressed conditions than under irrigated conditions at high values of *transp_eff_cf* highlight the role model setup can play on the effect of changing parameter values. The results from the 1st ratoon in Figure 2.4 are indicative of the effect *transp_eff_cf* can have on simulated yields and show that using different values of *transp_eff_cf* under irrigated and stressed conditions could affect simulated biomass yields. However, these results should not be considered definitive values for each variety.

A recent pot experiment using 20 sugarcane varieties identified statistically significant genetic variability in TE as well as significant interactions between genotype and water stress treatments (Jackson et al., 2014). On an above-ground biomass basis, Jackson et al. (2014) found that genetic variation in TE was statistically significant under water stressed conditions ($p<0.01$) but found only low statistical evidence ($p=0.12$) for variation under irrigated conditions. The sensitivity of simulated yields to *transp_eff_cf* values and the variability of *transp_eff_cf* values that best simulated variety yields suggest that including this genetic variation in TE in crop models would be beneficial. The results for TE strongly support the inclusion of other variety parameters in general. A better understanding of crop responses to water-limited conditions will improve the ability of crop models to simulate variety differences in specific environments. This will allow researchers to further investigate variety and environment interactions that are particularly important to breeding programs and are currently being explored in other commercial crop industries.

2.3.4. Limitations and future research

This chapter has considered a descriptive assessment of the simulation of varietal differences using APSIM-Sugar. The limited data set used was not appropriate for a more rigorous quantitative assessment. Experiments for a larger number of sites would allow researchers to more confidently interpret the results. This chapter also considered the effect of modifying TE within APSIM-Sugar as an example of the potential benefits of including new variety parameters. Other parameters that are important under water stressed conditions such as rooting depth and stomatal conductance (Inman-Bamber et al., 2012) should also be considered in future research. The results presented here suggest that variety parameter definitions within APSIM-Sugar are currently insufficient to accurately simulate yield differences between varieties and how different varieties respond to stress. While this chapter has focused on the sensitivity of simulation output to TE it will be necessary for future research to consider re-parameterising all variety parameters. A targeted sensitivity analysis would allow researchers to identify which variety parameters are most influential to model outputs. This will help guide field experiments by identifying what data needs to be collected to calibrate the model.

Where data are not available, statistical calibration of parameter values is a viable alternative. Descriptive data analysis identified *transp_eff_cf* parameter values that produced simulated yields closer to observed yields under stressed conditions. However, data were limited for individual varieties and several modifications were required to accurately simulate the observed field trials. These limitations reduce the applicability of the results to new scenarios such as new growing environments. Furthermore, the simulation of higher biomass under stressed conditions than irrigated conditions at high values of *transp_eff_cf* highlight that differences in parameter values may be influenced by limitations in the model.

Using a larger data set and appropriate calibration techniques it would be possible to statistically calibrate the *transp_eff_cf* parameter and other variety parameters within APSIM for each variety. Statistical calibration techniques have been used for sugarcane in the DSSAT-Canegro model (Marin et al., 2011) and for crop models of other commercial crops such as wheat (He et al., 2012) and rice (Iizumi et al., 2011). No attempt has been made to employ such techniques in APSIM-Sugar.

2.4. Conclusion

APSIM-Sugar simulations of the standard variety Q117 were within one standard error of observed mean yields for 4 commercially released varieties under irrigated and water stressed conditions after adjusting RUE and accounting for lodging in the irrigated treatment. However, a detailed comparison revealed that APSIM-Sugar was unable to simulate the observed differences between varieties yields and how these differences change when crops are grown under water stressed conditions. Modifying APSIM-Sugar's TE parameter (*transp_eff_cf*) had a large effect on simulated yields. For each variety, simulated yields were closer to mean observed yields for different values of *transp_eff_cf* under stressed conditions in the 1st ratoon. This suggests that APSIM-Sugar simulations could be improved by incorporating the latest physiological knowledge on genetic variation in TE and by extension, other 'new' variety parameters. To efficiently overhaul trait characterisations, future research will need to consider the sensitivity of simulation outputs to the full range of variety parameters in order to identify the traits that are most suited to closer examination. Where measured data on variety specific traits is unavailable statistical models can be used to calibrate model parameters. Models capable of variety simulation can be used to explore variety and environment interactions and help identify desirable variety traits. This will improve the crop model as a decision support system.

2.5. Chapter 2 Summary

The potential of crop modelling to aid farm management decisions has been demonstrated in the sugar industry. Models such as the Agricultural Production Systems sIMulator (APSIM) have been used in scheduling irrigation and fertilisation and for forecasting yields. APSIM models were developed based on variety parameters of a limited number of traits such as leaf area and how biomass is partitioned. Many of these variety parameters use the same value for all varieties because they have not been measured or defined for different genotypes. The varieties included in the model are no longer widely used for commercial applications and may not represent the genetic and phenological variability found in currently grown varieties. This could reduce the accuracy of simulated results for new varieties. To improve APSIM as a decision support system, deficiencies in APSIM's ability to simulate varietal differences should be identified.

The biomass yields of four commercially released sugarcane varieties that are currently defined within APSIM were simulated in this chapter. These varieties were also grown under water stressed and fully irrigated conditions at Home Hill over three years. An exploratory data analysis procedure compared simulated and observed differences between varieties. Simulated yields closely resembled observed yields if variety differences were ignored. However, APSIM did not contain many trait parameter differences between varieties and this limited the ability of APSIM to reproduce observed variety responses to water stress. To simulate these interactions effectively, varieties need to be accurately defined in the model.

A descriptive sensitivity analysis that varied the TE parameter (*transp_eff_cf*) in APSIM demonstrated how additional variety parameters can affect yield simulations. Incrementally adjusting *transp_eff_cf* had a large effect on simulated yields. Under stressed conditions, *transp_eff_cf* values as low as 0.0061 g kPa g^{-1} and as high as 0.0121 g kPa g^{-1} were required to closely simulate mean observed yields for different varieties assuming the difference response to water stress between varieties could be attributed solely to differences in TE. This varied from the default APSIM value of 0.0080 g kPa g^{-1}. This chapter illustrated the need for accurate characterisation of variety specific traits to improve simulation of variety performance in different environments. Future research must consider the effect of all variety specific parameters to identify which parameters have the greatest effect on simulated yields. Variety specific modelling can potentially be used to identify ideal varieties for specific environments and to tailor management strategies to specific combinations of varieties and environments.

Chapter 3

Global sensitivity analysis of key parameters in a process-based sugarcane growth model – A Bayesian approach

Relevant publication	Sexton, J., Everingham, Y., 2014. Global sensitivity analysis of key parameters in a process-based sugarcane growth model - A Bayesian approach, In: Ames, D.P., Quinn, N.W.T., Rizzoli, A.E. (Eds.), Proceedings of the 7th International Congress on Environmental Modelling and Software: San Diego, California, USA.
Statement of intellectual input from co-authors	Sexton and Everingham developed the research question. Sexton wrote the draft paper and Everingham provided editorial assistance. Sexton performed the data analysis and produced all figures and tables.
Publication status	Published

3.1. Introduction

Sugarcane crop models have been used as support tools for various management decisions. Lisson et al. (2005) reviewed the use of sugarcane crop models to optimize irrigation and harvest scheduling and perform yield forecasts. More recently crop models have been used to project climate change impacts on productivity and nutrient management (Biggs et al., 2013; Everingham et al., 2015). Research has also expanded into modelling variety specific traits that could improve yield under water stressed conditions (Inman-Bamber et al., 2012). This has the potential to guide the development of new cane varieties as well as improve irrigation management. Despite the potential advantages in variety simulations current sugarcane models such as the 'Sugar' module in the Agricultural Production System sIMulator (APSIM-Sugar; (Keating et al., 1999)) can struggle to simulate observed differences in biomass yields between varieties (Chapter 2).

The increasing use of crop models in climate change research and the potential impact that modelling can have on environmental and economic management decisions, requires researchers to quantify and analyse uncertainty in crop models. Sensitivity analysis in particular has been a recent focus of crop modelling entities such as AGMIP (Rosenzweig et al., 2013). Global sensitivity analysis investigates how uncertainty in a model input or group of inputs affects uncertainty in model outputs and can be used to identify input parameters that model outputs are sensitive to (Kennedy and O'Hagan, 2001).

Global sensitivity analysis considers substantial changes in input parameters. The variance induced in the output by changes in an input is averaged over the variance induced by all input parameters (Saltelli et al., 1999). Comparatively, local sensitivity analysis is based on partial derivatives of the function relating inputs to outputs at a central point, holding all other parameters constant. This represents slight changes to the input parameter values and may not reflect the true uncertainty in model parameters (Oakley and O'Hagan, 2004).

A range of methods exists for analysing crop model output sensitivity to model input parameters. These methods generally use a Monte Carlo approach, selecting a large number of random samples drawn from a prior distribution of the input parameter values. The Sobol scheme (Sobol, 1993) is an example of a Monte Carlo approach to global sensitivity analysis. The computational efficiency of such methods has been improved in such schemes as the extended-FAST method (Saltelli et al., 1999) but can still require thousands of simulations. This is generally impractical for computationally expensive models such as process–based crop models. A Bayesian approach to global sensitivity analysis using a Gaussian Process based emulator can be an efficient alternative (Oakley and O'Hagan, 2004; O'Hagan, 2006). Zhao et al. (2014) performed global sensitivity analysis on 10 parameters in the APSIM Wheat model for several study sites. Using the extended-FAST methodology this analysis required 10000 simulations per study site/treatment combination. Parry et al. (2013) performed a global sensitivity analysis on 11 parameters in an agent-based model for skylark populations. Using the Gaussian Process approach of Oakley and O'Hagan (2004) the analysis was conducted using only 200 simulation runs.

In this chapter the Bayesian approach to sensitivity analysis described by Oakley and O'Hagan (2004) as implemented in the freely available software GEM-SA (Kennedy, 2005) is used to asses the sensitvity of simulated biomass and sugar yields to 14 parameters in the APSIM-Sugar model. Knowledge of influential parameters will lead to a better understanding of the model and may lead to improved simulation of sugarcane under a range of environments.

3.2 The Gaussian Process Emulator

The Bayesian approach to global sensitivity analysis described by Oakley and O'Hagan (2004) is part of a range of Bayesian tools for model analysis referred to as Bayesian Analysis of Computer Code Output (O'Hagan, 2006). Here, the general approach to developing the emulator and performing sensitivity analysis as implemented in the GEM-SA (Gaussian Emulation Machine-Sensitivity Analysis) software package is outlined. Further details of the underlying mathematics can be found in Kennedy and O'Hagan (2001) and documentation in the GEM-SA software package (Kennedy, 2005). Crop model outputs ($\mathbf{Y}$) can be considered a function of model inputs ($\mathbf{X}$) (3.1). In the Bayesian sense the crop model $f(\mathbf{X})$ is assumed unknown and is thus considered a random function. A Gaussian distribution of functions is then used to represent our prior beliefs of $f(\mathbf{X})$ (3.2).

$$\mathbf{Y} = f(\mathbf{X}) \tag{3.1}$$

where:

$\mathbf{X} = [x_1, x_2, \ldots, x_p]$ and x_i is the i^{th} parameter of interest

$$[f(\mathbf{X})|\boldsymbol{\beta}, \sigma^2, \boldsymbol{r}] \sim N(m(\mathbf{X}), \mathrm{cov}(f(\mathbf{X}), f(\mathbf{X}'))) \tag{3.2}$$

where:

$$m(\mathbf{X}) = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p \tag{3.3}$$

$$\mathrm{cov}(f(\mathbf{X}), f(\mathbf{X}')) = \sigma^2 c(\mathbf{X}, \mathbf{X}') = \sigma^2 \exp\left(-\prod_{i=1}^{p} r_i (x_i - x_i')\right). \tag{3.4}$$

The prior distribution of any collection of outputs ($f(x_1) \ldots f(x_n)$) is multivariate normal with mean vector derived from (3.3) and covariance matrix derived from (3.4). The Gaussian distribution is mathematically convenient (Kennedy and O'Hagan, 2001) and has been proven effective for a range of emulation based analyses (Kennedy et al., 2006). Expressing the mean function as a linear additive model can be convenient for analysis but should be modified to reflect any beliefs about the structure of the simulator (Oakley and O'Hagan, 2004). The value σ^2 represents the overall variance about the mean function while r_i are unknown roughness parameters. Within the GEM-SA software package the unknown hyper-parameters $\boldsymbol{\beta}$ and σ^2 are given a constant joint prior probability $p(\boldsymbol{\beta}, \sigma^2) \propto \sigma^{-2}$. Each r_i is assumed to be independent with an $\exp(0.01)$ prior distribution.

Using a smooth correlation in the covariance is an advantage of this methodology. This implies that if $f(\mathbf{X})$ is known and $f(\mathbf{X})$ is close to $f(\mathbf{X}')$ we have some information about $f(\mathbf{X}')$. This provides extra information compared to Monte Carlo methods and can significantly reduce the number of simulations required. In comparison to the random draw from the prior parameter sample space used in Monte Carlo methods, model outputs ($\mathbf{Y}$) are observed at design points selected to efficiently cover the parameter sample space. Design points are selected by maximizing the minimum distance between points and/or minimizing the correlation between points. The GEM-SA software package can build a Maximin Latin Hypercube or LP-TAU design (Kennedy, 2005). It can then be shown that the emulator, conditional on $\boldsymbol{r}$ and $\mathbf{Y}$, has a posterior Student's t-distribution (3.5) with given posterior mean function $m^*(\mathbf{X})$ and posterior covariance $\hat{\sigma}^2 c^*(\mathbf{X}, \mathbf{X})$.

$$[f(\mathbf{X}) \mid \boldsymbol{r}, \mathbf{Y}] \sim t_{n-(p+1)}(m^*(\mathbf{X}), \hat{\sigma}^2 c^*(\mathbf{X}, \mathbf{X})) \tag{3.5}$$

Variance based sensitivity indices can be calculated from the posterior distribution. Of particular interest are the first order sensitivity index (S_i) and the total sensitivity index (ST_i) (Oakley and O'Hagan, 2004; Kennedy, 2005). The first order sensitivity index for x_i represents the expected reduction in output variance if x_i were known, i.e. an index of the effect that modifying x_i alone as on model outputs - the 'main effect' of x_i. The total sensitivity index represents the unexplained variance that would remain if all x_{-i} (all x other than x_i) were known and is a way of assessing the main effect of x_i and all higher order interactions to which x_i may contribute. Uncertainty in the parameter main effects on emulator outputs can also be calculated from the posterior distribution either analytically or through random draws from the posterior distribution.

3.3 The APSIM Sugarcane Growth Model and Key Parameters

APSIM-Sugar simulates important agronomic measures of crop productivity such as sugar yield, cane yield and sugar content of stalks (CCS) on a daily time step. These measures are derived from simulated crop biomass which is divided into leaf, cabbage, structural stem, roots and sucrose (Keating et al., 1999). The accumulation of biomass is driven largely by radiation use efficiency (RUE) where radiation refers to the 300 nm to 3000 nm bandwidth. RUE defines the ratio of biomass produced to intercepted radiation and can be limited by various environmental stresses such as temperature, water deficit or excess and nitrogen deficit.

There are five main categories of parameters in the APSIM-Sugar model that control how the crop grows given environmental and management conditions. These include constants, generic plant crop and ratoon crop parameters and variety parameters for plant and ratoon crops (http://www.apsim.info/Documentation/Model,CropandSoil/CropModuleDocumentation/Sugar.aspx). The growing environment is largely described by environmental parameters including climate parameters and soil parameters. Generic plant and ratoon parameters control growth and partitioning, water use and temperature and water stress factors. Eleven parameters are used to directly define a variety (Table 3.1). These parameters control leaf development (*leaf_*size, *tillerf_leaf_*size, *green_leaf_no*), partitioning of assimilates (*cane_fraction*, *sucrose_fraction_stalk*, *sucrose_delay*, *min_sstem_*sucrose, *min_sstem_sucrose_redn*) and phenological development based on thermal time (*tt_emerg_to_begcane*, *tt_begcane_to_flowering*, *tt_flowering_to_crop_end*) as described in Chapter 1.

Recent research has suggested that transpiration efficiency (TE) can vary between varieties and levels of water stress (Jackson et al., 2014). Rooting vigour, TE and stomatal conductance have been identified as possible traits that may lead to higher biomass yields under stressed conditions (Inman-Bamber et al., 2012). The root water extraction coefficient (k_L) has been used as a surrogate for stomatal conductance in APSIM-Sugar (Inman-Bamber et al., 2012).

Table 3.1. Key APSIM-Sugar parameters for use in sensitivity analysis

Parameter	Units	Representative Values
leaf_size	mm^2	55000 (maximum)
cane_fraction	$g\ g^{-1}$	0.70
sucrose_fraction_stalk	$g\ g^{-1}$	0.55
sucrose_delay	$g\ m^{-2}$	0
min_sstem_sucrose	$g\ m^{-2}$	400
min_sstem_sucrose_redn	$g\ m^{-2}$	10
tt_emerge_to_begcane	^{O}C day	1900
tt_begcane_to_flowering	^{O}C day	6000
tt_flowering_to_crop_end	^{O}C day	2000
green_leaf_no	leaves	13
tillerf_leaf_size	$mm^2\ mm^{-2}$	1.5 (leaf 6 and 10)
transp_eff_cf	$g\ kPa\ g^{-1}$	0.0087
rue	$g\ MJ^{-1}$	1.85 (plant) / 1.65 (ratoon)
k_L	nil	Varies with depth of roots

3.4. Methodology

3.4.1. Model initialization and parameter prior distributions

APSIM-Sugar environment and management settings were calibrated to simulate a breeding program at Home Hill in Queensland, Australia (Basnayake et al. (2012b); Chapter 2). Uniform prior distributions for 14 parameters were generated for the sensitivity analysis (Table 3.2). Ranges for variety parameters: *cane_fraction*, *sucrose_fraction_stalk*, *sucrose_delay*, *min_sstem_sucrose*, *tt_emerg_to_begcane*, *tt_begcane_to_flowering*, *tt_flowering_to_crop_end and tillerf_leaf_size* represent the range of parameter values reported for sugarcane varieties in APSIM-Sugar. Maximum and minimum values for *leaf_size* were selected to represent maximum leaf area values for a range of commercial varieties (Inman-Bamber, 2013). For simplicity *leaf_size* was modified relative to *leaf_size* for variety Q117 based on maximum leaf area. The range for parameters *green_leaf_no, rue* and k_L were adapted from data recorded as part of breeding field trials conducted under irrigated conditions at Home Hill, Queensland, Australia (Basnayake et al., 2012b). The range of values for parameter *green_leaf_no* were based on observed counts of green leaves for 89 varieties grown in the trial. Parameters *rue* and k_L were adjusted to represent observed variation of conductance under well irrigated conditions (*rue*) and the difference between well irrigated and stressed conditions (k_L). Adjustment factors for each of 89 varieties were calculated relative to variety Q117. For example, plant *rue* in APSIM is by default 1.8 g MJ^{-1}. If variety X had a *rue* adjustment factor of 0.90, *rue* for variety X was modified to 1.62 g MJ^{-1}. Adjustment factors for k_L were applied to all soil layers. For example, consider the first three layers of a soil with a defined k_L of [0.010 0.050 0.100] for depths down to [15 cm 30 cm 45 cm] respectively. If variety X had a k_L adjustment factor of 0.9, the k_L for the first three layers of variety X would be [0.009 0.045 0.090].

Observed *rue* adjustments did not exceed 1.1 (1.98 g MJ^{-1}). This remains consistent with sugarcane literature which suggests a maximum rue of approximately 2 g MJ^{-1} (Muchow et al., 1996b). Inman-Bamber et al. (2012) suggested a reduction in k_L of up to 50% was not unrealistic. However, as k_L is often defined for individual soils (Inman-Bamber et al., 2000), the range of k_L adjustment factors may approach inappropriate values for some soil types and care should be taken in interpreting resultant calibrations.The range for *transp_eff_cf* was selected based on transpiration rates recorded in a greenhouse study under irrigated and water stressed conditions (Jackson et al. 2014) and matched those used in Chapter 2. Values for *transp_eff_cf* were based on irrigated and stressed conditions in order to capture the possibility of higher *transp_eff_cf* values under brief periods of water stress that may occur even under well irrigated conditions.

Table 3.2. Uniform parameter ranges used for sensitivity analysis.

Parameter	Units	Minimum	Maximum
leaf_size (maximum)	mm^2	20000	70000
cane_fraction	$g\ g^{-1}$	0.65	0.80
sucrose_fraction_stalk	$g\ g^{-1}$	0.4	0.7
sucrose_delay	$g\ m^{-2}$	0	600
min_sstem_sucrose	$g\ m^{-2}$	400	1500
min_sstem_sucrose_redn	$g\ m^{-2}$	9	11
tt_emerg_to_begcane	^{O}C day	1200	1900
tt_begcane_to_flowering	^{O}C day	5400	6600
tt_flowering_to_crop_end	^{O}C day	1800	2200
green_leaf_no	leaves	9	15
tillerf_leaf_size	$mm^2\ mm^{-2}$	1	6
transp_eff_cf	$g\ kPa\ g^{-1}$	6.0	14.0
rue[1] (adjustment factor)	nil	0.74	1.08
k_L[2] (adjustment factor)	nil	0.57	1.81

[1] rue was adjusted relative to APSIM default values so that 1 relates to the APSIM default rue of 1.8 g MJ^{-1} (plant) and 1.65 g MJ^{-1} (ratoon)

[2] k_L was adjusted relative to APSIM default values based on APSIM Q117 and soil data. A value of 1 represents the default value for all soil layers.

3.4.2. Sensitivity analysis

The GEM-SA software package (Kennedy, 2005) was used to perform global sensitivity analysis on simulated biomass (g m^{-2}) and sucrose yield (g m^{-2}) at harvest for a first ratoon crop under irrigated and water stress conditions (a total of 4 simulation outputs assessed). The Maximin Latin Hypercube approach was used to create a design of 400 points that efficiently covered the 14 dimensional parameter space. The maximum value of 400 points was used to provide the most rigorous analysis possible. A Gaussian Process emulator was developed for each of the 4 simulation outputs separately.

Twenty percent of the design was left out for validation to assess uncertainty in the emulator results. To further quantify uncertainty a 95% credible interval on all main effects was produced from 1000 random draws from the emulator posterior distribution. Plots of the emulator mean of the main effects from 1000 random draws were used to visualise the response of outputs to each of the 14 variables. Finally first order sensitivity indices and total sensitivity indices were recorded for each variable for all simulation outputs. A high S_i indicated an influential parameter.

3.5. Results

3.5.1. Sensitivity analysis

The mean main effects of 1000 draws from the posterior emulator are plotted for biomass in Figure 3.1 and sucrose yield in Figure 3.2. First order sensitivity indices (S_i) and total sensitivity indices (ST_i) are recorded in Table 3.3. Most notably *tt_begcane_to_flowering*, *tt_flowering_to_crop_end*, *min_sstem_sucrose_redn* and *tillerf_leaf_size* had S_i indices less than 1 for all outputs. Similarly biomass yields were insensitive to parameters related to sucrose (*sucrose_fraction_stalk, sucrose_delay, min_sstem_sucrose*). The number of green leaves parameter (*green_leaf_no*) was the most influential of the standard APSIM-Sugar variety parameters. Simulated biomass and sucrose yields were most sensitive to changes in *rue* under irrigated conditions and *transp_eff_cf* under stressed conditions. Plots of main effects suggested model output sensitivity can be non-linear and change dramatically under irrigated or water stressed conditions.

Table 3.3. Variance based sensitivity measures for biomass and sucrose yields at harvest under irrigated and water stressed conditions. The first order sensitivity indices (S_i) represent the percentage of total variance contributed by each parameter. The total sensitivity indices (ST_i) reflect the influence of each parameter and its contribution to any interactions.

Parameter	Biomass at Harvest				Sucrose yield at Harvest			
	Irrigated		Stressed		Irrigated		Stressed	
	S_i	ST_i	S_i	ST_i	S_i	ST_i	S_i	ST_i
leaf_size (maximum)	12.24	13.17	1.08	1.79	7.89	9.70	1.23	1.92
cane_fraction	4.90	5.65	5.32	5.83	1.61	2.20	4.51	5.24
sucrose_fraction_stalk	0.06	0.07	0.01	0.05	10.30	11.65	8.53	9.92
sucrose_delay	0.00	0.00	0.00	0.00	1.41	2.84	0.28	0.60
min_sstem_sucrose	0.10	0.12	0.00	0.00	10.02	12.32	12.80	13.95
min_sstem_sucrose_redn	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.12
tt_emerg_to_begcane	0.01	0.43	0.07	0.10	1.56	2.87	2.50	3.24
tt_begcane_to_flowering	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01
tt_flowering_to_crop_end	0.00	0.02	0.00	0.13	0.02	0.05	0.00	0.19
green_leaf_no	19.87	21.23	8.42	10.25	14.42	15.41	11.38	12.28
tillerf_leaf_size	0.17	1.04	0.04	0.73	0.05	0.29	0.01	0.15
transp_eff_cf	3.04	5.66	70.65	73.51	0.33	1.94	35.15	39.87
rue	54.05	56.28	7.56	9.22	44.93	49.00	16.26	19.58
k_L	1.09	2.81	2.83	3.73	0.27	2.07	0.57	2.01

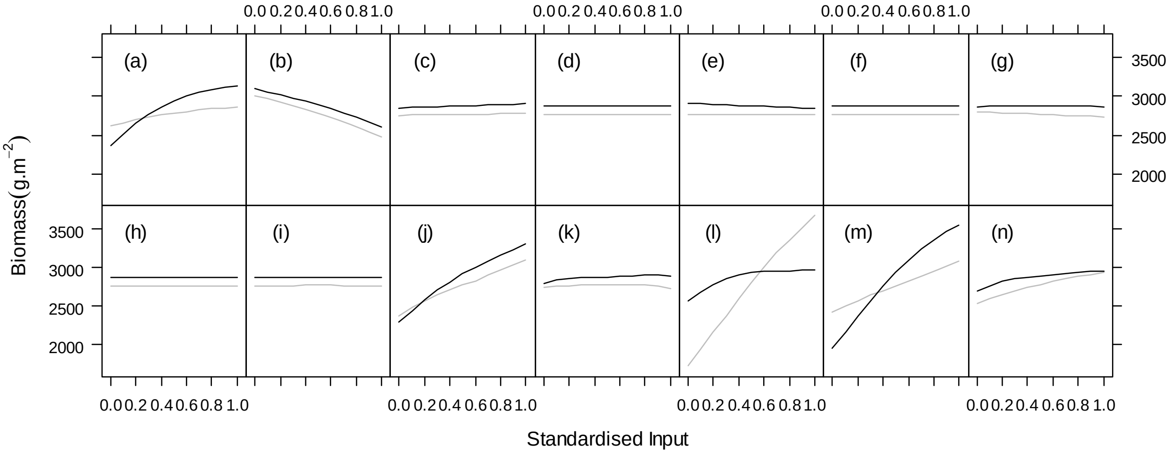

Figure 3.1. Parameter main effect on biomass under irrigated (black) and stressed (grey) conditions. Effects recorded for (a) *leaf_size*, (b) *cane_fraction*, (c) *sucrose_fraction_stalk*, (d) *sucrose_delay*, (e) *min_sstem_sucrose*, (f) *min_sstem_sucrose_redn*, (g) *tt_emerge_to_begcane*, (h) *tt_begcane_to_flowering*, (i) *tt_flowering_to_crop_end*, (j) *green_leaf_no*, (k) *tillerf_leaf_size*, (l) *transp_eff_cf*, (m) *rue* and (n) k_L. Input values are standardized as 0 = minimum value and 1 = maximum value from Table 3.1.

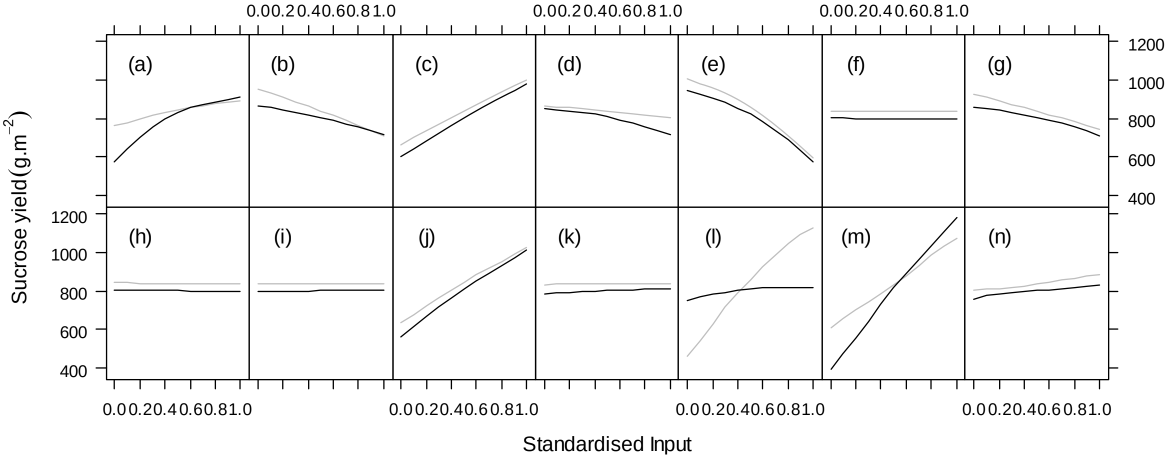

Figure 3.2. Parameter main effect on sucrose yield under irrigated (black) and stressed (grey) conditions. Effects recorded for (a) *leaf_size*, (b) *cane_fraction*, (c) *sucrose_fraction_stalk*, (d) *sucrose_delay*, (e) *min_sstem_sucrose*, (f) *min_sstem_sucrose_redn*, (g) *tt_emerge_to_begcane*, (h) *tt_begcane_to_flowering*, (i) *tt_flowering_to_crop_end*, (j) *green_leaf_no*, (k) *tillerf_leaf_size*, (l) *transp_eff_cf*, (m) *rue* and (n) k_L. Input values are standardized as 0 = minimum value and 1 = maximum value from Table 3.1.

3.5.2. Emulator accuracy

Standardized validation root mean square errors (RMSE), largest roughness parameters and largest standardized errors were recorded (Table 3.4). Standardized validation RMSE reflects the overall performance of the emulator in reproducing the APSIM-Sugar model outputs and should be close to 1. Standardized validation RMSE values larger than 1 indicate emulator outputs overestimated APSIM-Sugar outputs while lower values indicate that emulator outputs underestimated APSIM-Sugar outputs. Roughness parameters indicate how non-linear the relationship between output and input parameters are. Input parameters with high roughness parameter values generally require more learning data points to accurately emulate the relationship, reducing the emulator efficiency (O'Hagan, 2006). Standardized errors are calculated for each of the training points and should be close to zero. Training points with standardized error values larger than 2 indicated poor emulation for that case and may be used to help identify regions of the design space for which the emulator performs poorly. Validation root mean squared standardized errors were all close to 1 with the greatest deviation occurring for simulated biomass under water stressed conditions. Roughness parameters were also relatively low. The largest roughness parameters were related to k_L and *rue* under irrigated conditions and *transp_eff_cf* under stressed conditions. The largest standardized errors were greater than 2 for all treatment/output combinations indicating that some cases were poorly reproduced by the emulator and may suggest that more training data was needed. Credible intervals (95%) on the parameter main effects on model outputs (based on 1000 random draws from the emulator posterior distribution), suggested that any uncertainty in the emulator did not result in a large uncertainty in emulator outputs and parameter main effects on those outputs (data not shown).

Table 3.4. Emulator performance statistics for biomass and sucrose yield at harvest under irrigated and water stressed conditions. Standardized RMSE should be close to 1 with larger values indicating an overestimation and lower values representing an underestimation. Smaller roughness parameters are desirable. Standardized errors of less than 2 are desirable.

Error Measure	**Biomass at Harvest**		**Sucrose at Harvest**	
	Irrigated	**Stressed**	**Irrigated**	**Stressed**
Validated RMSE (standardized)	1.13	1.57	0.99	1.22
Largest Roughness Parameter	3(*rue*, k_L)	3.33(*transp_eff_cf*)	3(*rue*, k_L)	4.15(*transp_eff_cf*)
Largest Standardized Error	3.00	5.56	2.74	3.33

3.6. Discussion

Emulator uncertainties were relatively low however the higher roughness parameters suggest close attention should be paid to *transp_eff_cf*, *rue* and k_L parameters. Emulator results for *transp_eff_cf* replicated the results found in Chapter 2 supporting the emulators' ability to accurately represent the model. Emulator accuracy would no doubt be further improved if non-influential parameters were removed from the analysis. This would allow the 400 design points to better cover the reduced parameter space.

The insensitivity of model outputs to *tt_begcane_to_flowering* and *tt_flowering_to_crop_end* is not surprising as these parameters are not currently implemented by APSIM-Sugar (Keating et al., 1999). These parameters were only included in this analysis as they are still listed as variety parameters in the APSIM-Sugar model yet no published work has looked at their role in simulations since (Keating et al., 1999). It is an important result then that these parameters are in fact not influencing simulation output. The insensitivity of simulated biomass to sucrose parameters is also to be expected. The lack of influence of *tillerf_leaf_size* and *min_sstem_sucrose_redn* are of greater import. Tillering is considered a desirable trait which can improve biomass yields and the low sensitivity of simulated biomass to *tillerf_leaf_size* is counterintuitive. It is important that future research investigates how *tillerf_leaf_size* is used by sugarcane modellers. For purposes of model calibration *tillerf_leaf_size* and *min_sstem_sucrose_redn* may be ignored, reducing the risk of over parameterisation when availability of observed data is low.

The influence of *leaf_size* on model outputs was distinctly non-linear under irrigated conditions (Figure 3.1 (a) and Figure 3.2 (a)). The plateau at higher values suggests that beyond a certain point increase in *leaf_size* will not increase yields. This is an important result in understanding how the model can be used for different sugarcane industries. For example, modelling differences in leaf area will have a greater impact for industries such as Australia that use varieties with smaller leaf areas, compared to industries such as Brazil where sugarcane varieties generally have larger leaf areas. For simulated biomass there was a marked difference in the influence of *rue* between irrigated and stressed conditions (Figure 3.1 (m)). This may mean that use of *rue* in variety parameterisations could affect simulations of variety by environment interaction. While *rue* was more influential under irrigated conditions, k_L was slightly more influential under stressed conditions. Although these two parameters do not vary in APSIM-Sugar by default, calibration of each may lead to a better simulation of environmental response.

Sugarcane industries are continually developing new varieties to improve productivity. In order to remain a relevant decision support tool models such as APSIM-Sugar must continually be updated to reflect current varieties and physiological knowledge. Unfortunately collecting the data on variety traits can be expensive and time consuming. Knowledge of influential model parameters can be used to evaluate the trade-off between the expense of measuring a particular trait to inform a crop model and the potential contribution the knowledge will make towards improving the simulation. The results from this study should be considered along with the expense of measuring relevant traits and the genetic heritability of traits when data is collected to inform crop models.

The use of a Gaussian Process to emulate the APSIM-Sugar model provided an efficient and effective global sensitivity analysis. For this analysis 800 simulations in APSIM-Sugar were required (400 parameter sets * 2 treatments). By comparison the extended-FAST method as implemented by Zhao et al. (2014), would have required as many as 28000 simulations in APSIM-Sugar (1000 parameter sets * 14 parameters * 2 treatments). In future emulator accuracy could be improved by removing parameters found to have negligible influence on key agronomic parameters. Improvements could also be made if more realistic information of the prior parameter distributions were identified and incorporated into the analysis. Currently the GEM-SA software allows for only uniform *or* normal prior distributions. Incorporating different prior distributions, when known, may affect the results. Furthermore when uniform distributions are used, the range used will affect the results. For example, a change in *leaf_size* was more influential at lower values (Figure 3.1(a)). Reducing the prior distribution of *leaf_size* to lower values could potentially increase the relative influence of *leaf_size*. This methodology could be extended to include other likely influential parameters at a wider range of environments and crop classes to assess potential interactions. Future research should also consider interactions between influential parameters.

3.7. Conclusion

The GEM-SA package was able to efficiently perform a global sensitivity analysis for the APSIM-Sugar model. While there was room for improvement in the choice of parameters and possibly the parameter prior distributions, the emulator was able to reproduce sensitivity results for TE previously produced using only the APSIM-Sugar simulator and was able to give some insight into likely influential and negligible variety parameters. In particular phenology parameters (e.g. tt_begcane_to_flowering), *tillerf_leaf_size* and *min_sstem_sucrose_redn* had little to no influence on either model output. Both model outputs were sensitive to parameters *rue*, *green_leaf_no* and *leaf_size* under irrigated conditions and *transp_eff_cf* under water stressed conditions. The most influential sucrose specific parameters were *sucrose_fraction* and *min_sstem_sucrose*. Identifying influential parameter values is the first step to improving variety specific simulations. The results of this analysis could be used to guide the calibration of the

APSIM-Sugar model so that new varieties are properly represented in model simulations. Such variety calibration could greatly impact APSIM-Sugar's ability as a decision support tool in the future.

3.8. Chapter 3 Summary

While several statistical methods are available to analyse model sensitivity, their application to complex process-based models is often impractical due to the large number of simulation runs required. A Bayesian approach to global sensitivity analysis can greatly reduce the number of simulation runs required by building an emulator of the model which is less computationally demanding. In this chapter a Gaussian Process emulator was used to efficiently assess the sensitivity of key agronomic outputs from the APSIM-Sugar crop model to influential input parameters. The sensitivity of simulated biomass and sucrose yield at harvest was assessed on 14 parameters representing varietal differences and growth response to water stress. Analysis was performed under irrigated and water stressed conditions. Simulated biomass and sucrose yield were found to be insensitive to 4 of the parameters tested (*min_sstem_sucrose_redn*, *tt_begcane_to_flowering*, *tt_flowering_to_crop_end* and *tillerf_leaf_size*) under both irrigated and stressed conditions. Both outputs were most sensitive to radiation use efficiency under irrigated conditions and transpiration efficiency under stressed conditions. Output sensitivity was often non-linear and for a given parameter, could vary between well irrigated and water stressed conditions. Understanding how these parameters affect simulation outputs and which parameters are most influential can help improve simulations of interactions between sugarcane varieties and growing environments. This in turn can help better guide management decisions in the future. The Bayesian approach to sensitivity analysis provided insight into influential and negligible model parameters.

Chapter 4

A dual method evaluation of the use of two Bayesian techniques for the calibration of variety parameters in a sugarcane crop model

Relevant publication	Sexton, J., Everingham, Y., Inman-bamber, G., 2015. A dual method evaluation of the use of two Bayesian techniques for the calibration of variety specific trait parameters in a sugarcane crop model. Environmental Modelling & Software, (submitted).
Statement of intellectual input from co-authors	The research question was developed with input from Sexton, Everingham and Inman-Bamber. Inman-Bamber provided methodology for developing prior parameter distributions. Sexton wrote the draft of the paper which was revised with input from Everingham and Inman-Bamber. Sexton performed data analysis and produced all figures and tables.
Publication status	Submitted

4.1. Introduction

Australian sugarcane varieties have changed over the last 15 years yet their representation in crop growth models has not. The Australian sugar industry is constantly developing new varieties to improve sucrose yield, pest and disease resistance and tolerance of abiotic stresses such as drought and water logging. Diseases such as orange rust (Magarey et al., 2001) have greatly affected prominent varieties like Q124, requiring new disease resistant varieties for commercial applications. Most varieties commonly grown in 1999 have been superseded by new varieties (Figure 4.1). Despite this crop models such as the Agricultural Production Systems sIMulator (APSIM) (Holzworth et al., 2014) do not offer options for these new varieties (APSIM-Sugar Version 7.5 r3124) (Keating et al., 1999). This has limited the ability of modellers to explore sugarcane varietal differences through simulation. In contrast, the ability to simulate varietal differences has been well explored in a range of other commercial crop industries. For example varietal simulations have been used to identify ideal varieties for given environments in crops such as peanuts (Putto et al., 2013), wheat (Laurila et al., 2012), and rice (Aggarwal et al., 1997); to investigate likely sources of genetic gains in soybeans (Boote et al., 2001) and to link crop models with genetic models (Chapman, 2008).

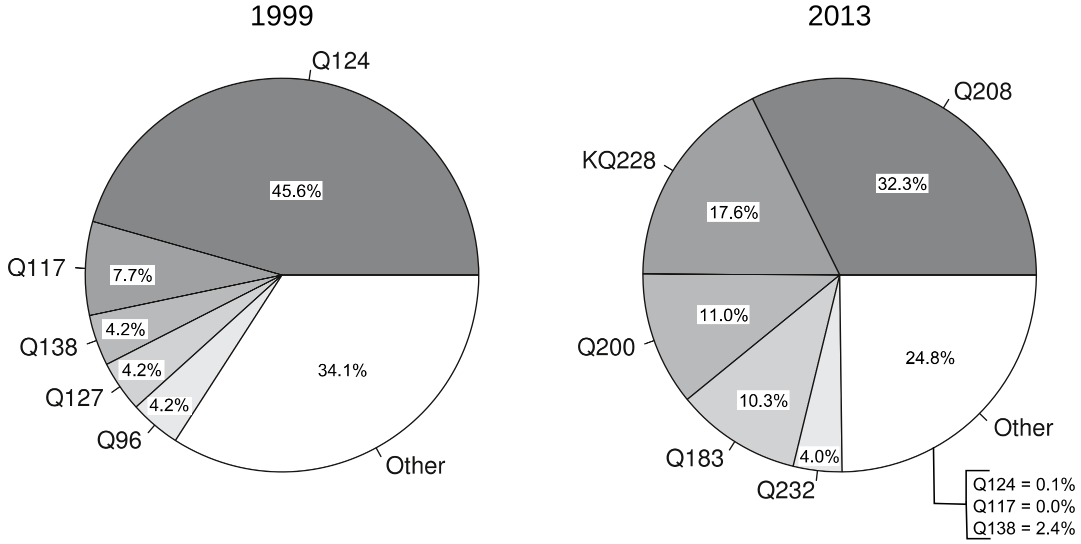

Figure 4.1. Percentage of hectares grown by variety in Australia (QLD and NSW) for 1999 and 2013. Values downloaded from QCANESelect™ provided by Sugar Research Australia (accessed 11-09-2014). Data were collected as part of the SPIDNet database (Lethbridge and Cox, 2010).

Dynamic (process-based) crop models are advantageous as they simulate the underlying physiological processes required to grow a crop (Lisson et al., 2005). Cropping-system simulators model crop growth in response to environments, soils, stresses, varieties and management decisions. Many such models are available for sugarcane including APSIM-Sugar, DSSAT-Canegro (Singels et al., 2008), QCane (Liu and Bull, 2001), AUSCANE (Jones et al., 1989) and STICS-Sugarcane (Brisson et al., 2003). These models are widely used as decision support tools to help identify industry best practices as well as helping farmers develop site specific management plans. DSSAT-Canegro and APSIM-Sugar are two of the most widely used models. For example APSIM-Sugar has been used in Australia for irrigation scheduling (Everingham et al., 2002), investigating nitrogen best management practices (Thorburn et al., 2010; Stewart et al., 2006; Skocaj et al., 2013), and climate change impact studies (Biggs et al., 2013; Webster et al., 2009). Canegro in the DSSAT environment has been used for similar studies largely in South Africa (Bezuidenhout et al., 2002; van der Laan et al., 2011; McGlinchey and Inman-Bamber, 1996; Jones et al., 2014) but also for climate change impacts in Swaziland (Knox et al., 2010) and Australia and Brazil (Singels et al., 2013). To date little research has considered varietal effects on such decision support research in sugarcane.

Canegro (DSSAT V4.5) represents 13 sugarcane varieties using 22 variety parameters while APSIM contains 14 sugarcane varieties described using 13 parameters. Some parameters representing physiological traits such as leaf area and number of green leaves can be quite easily measured. However, accurately obtaining parameters for other traits (e.g. transpiration efficiency) can be costly and time consuming. An alternative approach is to estimate parameters that represent traits that are difficult to measure, from knowledge about traits that are routinely or more easily measured such as biomass or sucrose accumulation. Makowski et al. (2006a) provides an overview of the various methods used to estimate crop model parameters such as sensitivity analysis, least squares regression and maximum likelihood. Recently more complex statistical approaches such as genetic algorithms (Mitchell, 1999) and Bayesian statistical approaches such as Generalized Likelihood Uncertainty Estimation (GLUE; (Beven and Binley, 1992)) and Markov Chain Monte Carlo (MCMC;(Gelman et al., 1997)) have found widespread application.

Bayesian statistical parameter estimation techniques like GLUE and MCMC allow researchers to use various sources of data and prior knowledge about likely parameter values. GLUE has become widely used in a range of crop models because it is relatively computationally simple (Makowski et al., 2002). GLUE has been used effectively for parameterizing generic crop models (Wang et al., 2005), models for maize (He et al., 2010), wheat (Mo and Beven, 2004), cotton (Pathak et al., 2012) and sugarcane (Marin et al., 2011). MCMC algorithms have been used to estimate crop model variety parameters for rice (Iizumi et al., 2011; Iizumi et al., 2009), maize (Tao et al., 2009), wheat (Tao and Zhang, 2013; Dumont et al., 2014) and soybeans (Archontoulis et al., 2014) but have not been applied to sugarcane crop models.

This chapter evaluates the use of GLUE and MCMC as tools to estimate sugarcane variety parameters in the APSIM-Sugar model. These Bayesian techniques allow researchers to make use of a range of prior knowledge about parameter values providing an advantage over other forms of parameter estimation. While GLUE has previously been applied to DSSAT-Canegro (Marin et al., 2011), neither GLUE nor MCMC has been applied to APSIM-Sugar. If applicable, Bayesian parameter estimation will provide a much needed systematic method for updating variety parameters for new varieties as they are developed. Keeping APSIM-Sugar up to date with commercially released varieties will allow crop modellers to investigate interactions between variety, environment and farm management practices and will help improve the model as a decision support tool.

4.2. Theory

4.2.1. Agricultural Production System Simulator

The APSIM-Sugar module simulates biomass accumulation on a daily time step (Keating et al., 1999). Biomass accumulation is driven largely by radiation through radiation use efficiency (RUE) and is divided into five live pools (leaf, cabbage, structural stem, roots and sucrose). Biomass accumulation is limited by low or high temperature, excess or deficit water stresses and nitrogen deficit effects on RUE (Singels, 2013). This allows APSIM to simulate differences between potential and attainable yields and hence benchmark production based on yield actually obtained (Inman-Bamber, 2013). From biomass, key productivity measures such as cane yield, sugar yield and sugar content of stalks (CCS), are simulated. The underlying biophysical processes and responses to imposed stress are defined by a range of model parameters.

Parameters that represent the biophysical processes of the sugarcane are divided into soil and climate parameters, generic plant and ratoon parameters and variety parameters. Table 4.1 lists a range of key parameters that define canopy development (parameters 1, 2, 12, 13 and 14), biomass partitioning (parameters 3-8) and phenological stages (parameters 9-11). Some physiological traits are represented by combinations of parameters such as the leaf size profile. Parameters *leaf_size* (area of fully expanded leaf) and *leaf_size_no* (leaf position along stalk) affect canopy development by describing inflection points of a Gompertz curve (Inman-Bamber, 2013). Parameters *sucrose_fraction_stalk* and *stress_factor_stalk* reflect how stress effects the partitioning of assimilates into sucrose (Keating et al., 1999). Although parameters 1-14 listed in Table 4.1 are classed as variety specific parameters in APSIM-Sugar, currently defined varieties differ only in fully expanded area of leaves and partitioning of biomass to sucrose in the stalk. Flowering in sugarcane is sporadic and variety parameters for phenology traits such as flowering, although available are not implemented (Keating et al. (1999); Chapter 2). Transpiration efficiency (TE) in sugarcane has recently been shown to vary between varieties (Jackson et al., 2014) but the corresponding parameter in APSIM-Sugar (*transp_eff_cf*) remains a constant for different varieties. In the DSSAT-Canegro model RUE has a corresponding variety specific parameter (Marin et al., 2014; Marin et al., 2011) but is generally considered a constant in APSIM-Sugar. Apart from the Marin et al. publications there is no published evidence for genetic variation in this trait which is difficult to measure and has a profound effect on crop productivity.

Table 4.1. APSIM-Sugar parameters: Parameters 1 to 14 are considered variety specific in the APSIM-Sugar model. Parameters represent morphological traits such as leaf size, and number of green leaves, while others represent developmental stages (parameters 9, 10 and 11), physiological traits such as RUE (parameter 16) or partitioning between sucrose and biomass (parameters 3 and 4). Some traits are described using combinations of variables such as the leaf size profile which is described using parameters *leaf_size* (parameter 1) and *leaf_size_no* (parameter 2).

Parameter	Description	Units	Values (Variety Q117)
1 *leaf_size*	Area of each leaf	mm^2	1500 55000 55000
2 *leaf_size_no*	Leaf number from top leaf	leaf	1 14 20
3 *cane_fraction*	Fraction of accumulated biomass partitioned to cane	g g^{-1}	0.70
4 *sucrose_fraction_stalk*	Fraction accumulated biomass partitioned to sucrose	g g^{-1}	1 0.55
5 *stress_factor_stalk*	Stress factor for sucrose accumulation	nil	0.2 1.0
6 *sucrose_delay*	Sucrose accumulation delay	g	0
7 *min_sstem_sucrose*	Minimum stem biomass before partitioning to sucrose commences	g	800
8 *min_sstem_sucrose_redn*	Reduction to minimum stem sucrose under stress	g	10
9 *tt_emerg_to_begcane*	Thermal time required from emergence to start stalk growth	°C d	1900
10 *tt_begcane_to_flowering*	Thermal time required from start of stalk growth to start of flowering	°C d	6000
11 *tt_flowering_to_crop_end*	Thermal time from flowering to crop death	°C d	2000
12 *green_leaf_no*	Green leaf number	leaves	13.0
13 *tillerf_leaf_size*	Expansion factor applied to leaf size due to tillering	nil	1 1 1.5 1 1
14 *tillerf_leaf_size_no*	Leaf number from top leaf	leaf	1 4 10 16 26
15 *transp_eff_cf*	Intrinsic transpiration efficiency coefficient	g kPa g^{-1}	0.0080
16 *rue*	Radiation use efficiency	g MJ^{-1}	1.8 (plant) 1.65 (ratoon)
17 k_L	Root water extraction coefficients	d^{-1}	Varies with soil

4.2.2. Bayesian statistical parameter estimation

Bayes' rule (4.1) relates prior belief about parameter values before observing any data (prior probability; $P(\boldsymbol{\theta})$), to posterior beliefs (posterior probability; $P(\boldsymbol{\theta}\,|\,\mathbf{Y})$) after observations are made through a sampling distribution known as the likelihood function ($P(\mathbf{Y}|\boldsymbol{\theta})$) (Gelman et al., 1997). That is, Bayes' rule defined as:

$$P(\boldsymbol{\theta}\,|\,\mathbf{Y}) \propto P(\boldsymbol{\theta})\, P(\mathbf{Y}|\boldsymbol{\theta}) \tag{4.1}$$

here:

$\boldsymbol{\theta}$ = a vector of p unknown parameter values: $\boldsymbol{\theta} = [\theta_1, \theta_2, \ldots, \theta_p]$;
$\mathbf{Y}$ = a vector of o observations: $\mathbf{Y} = [y_1, y_2, \ldots, y_o]$;
$P(\boldsymbol{\theta})$ = the joint prior distribution of unknown parameters;
$P(\mathbf{Y}|\boldsymbol{\theta})$ = the likelihood function and
$P(\boldsymbol{\theta}|\mathbf{Y})$ = the joint posterior distribution of unknown parameters,
provides a systematic method of updating our beliefs of the parameter probability as more observations are made.

The likelihood function $P(\mathbf{Y}\,|\,\boldsymbol{\theta})$ describes the probability of the data $\mathbf{Y}$ given the parameters $\boldsymbol{\theta}$, dependant on the probability distribution of model errors – the difference between observed and simulated values (Makowski et al., 2006a). In the case of parameter estimation the parameters are the unknown quantity of interest and the likelihood function is generally defined as $L(\boldsymbol{\theta}|\mathbf{Y})$, that is the likelihood of parameter set $\boldsymbol{\theta}$ given observations $\mathbf{Y} = [y_1, y_2, \ldots, y_o]$ with model error variance (σ^2). The choice of likelihood function should reflect the actual distribution of model errors (He et al., 2010; Stedinger et al., 2008; Makowski and Wallach, 2002).

Most widely used likelihood functions for both GLUE and MCMC are based on the Gaussian distribution such that:

$$L(\boldsymbol{\theta}|\mathbf{Y}) = \prod_{o=1}^{O} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{[y_o - \hat{y}_o(\boldsymbol{\theta})]^2}{2\sigma^2}\right) \tag{4.2}$$

where:

y_o is the o^{th} observation and
$\hat{y}_o(\boldsymbol{\theta})$ is the o^{th} simulated value using parameter set $\boldsymbol{\theta}$,
assuming that model errors (residuals) are normally distributed (Jones et al., 2011; Marin et al., 2011; He et al., 2010; Iizumi et al., 2009; Makowski et al., 2006a; Pathak et al., 2012; Dumont et

al., 2014; Makowski et al., 2002). Model error variance can be estimated by the variance in the observations or from a well calibrated example (Pathak et al., 2012; Wang et al., 2005). Furthermore error variance σ^2 may be specified for each observation (σ_o^2) if variances for each are known (Iizumi et al., 2009).

In the examples of crop model calibrations mentioned here, model errors are generally assumed to be normally distributed without reporting whether this assumption is valid (Jones et al. 2011; Marin et al., 2011; Iizumi et al., 2009; Pathak et al., 2012). In practice observations often used to calibrate crop models such as biomass or leaf area index (LAI) may have variances that change with the size of the observation (Wallach et al. 2011). A particular example is the use of measurements of the same crop at different times during the growing season. The assumption of normality in such cases may be addressed by performing the calibration using appropriately transformed (e.g. log transformed) observations (Wallach et al., 2011; Kennedy and O'Hagan 2001). Dumont et al. (2014) addressed this issue by using a modified likelihood function in an MCMC based calibration of the STICS crop model. In that study Dumont et al. (2014) replaced the error variance with a coefficient of variation calculated as the ratio of the standard deviation and the value of the observation. Not properly representing the error variance can lead to higher uncertainty in the parameter posterior distributions and poor performance of calibrated models for situations not used in the calibration. The likelihood based on a normal distribution is used in this chapter as it has been used effectively in similar studies such as Marin et al. (2011).

The main advantage of the Bayesian approach to parameter estimation is that prior knowledge of parameter values is taken into account to describe a posterior probability based on observations. This allows researchers to estimate parameters from different data sources and quantify the uncertainty in model outputs due to parameter uncertainty (Makowski et al., 2006a). Uniform priors are generally used with ranges based on published data or wide enough to be relatively sure of capturing the true parameter value (Beven and Binley, 1992). However, prior distributions should be defined to capture any known distribution and covariance between parameters.

4.2.2.1. Generalized Likelihood Uncertainty Estimation

GLUE (Beven and Binley, 1992; Beven and Freer, 2001; Stedinger et al., 2008) is a Monte Carlo approach whereby a large sample of parameter sets $[\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots, \boldsymbol{\theta}_Q]$ are chosen from a defined prior distribution. A goodness-of-fit likelihood is calculated for each parameter set and used to produce weighted posterior probability densities for each parameter set which in turn are used to approximate the posterior distribution for each parameter. A simplistic overview can be outlined in four steps:

1. A prior probability distribution is developed for each parameter
2. A Monte Carlo approach is used to generate a large number (Q) of random samples of parameter sets from the prior distribution
3. Calculate likelihood $L(\boldsymbol{\theta}_i|\mathbf{Y})$ for each parameter set using an explicit likelihood function
4. Calculate the posterior probability density $p(\boldsymbol{\theta})$ of each parameter set (Jones et al., 2011; He et al., 2010) as:

$$p(\boldsymbol{\theta}_i) = \frac{L(\boldsymbol{\theta}_i|\mathbf{Y})}{\sum_{i=1}^{Q} L(\boldsymbol{\theta}_i|\mathbf{Y})} \tag{4.3}$$

Posterior probability densities can then be used to define the empirical posterior distribution and the distribution mean:

$$\hat{\boldsymbol{\mu}}_{post} = \sum_{i=1}^{Q} p(\boldsymbol{\theta}_i)\cdot\boldsymbol{\theta}_i \tag{4.4}$$

and variance:

$$\hat{\boldsymbol{\sigma}}^2_{post} = \sum_{i=1}^{Q} p(\boldsymbol{\theta}_i)\cdot(\boldsymbol{\theta}_i - \hat{\boldsymbol{\mu}}_{post})^2 \tag{4.5}$$

for each parameter.

GLUE is often referred to as a pseudo-Bayesian approach as the likelihood function $L(\boldsymbol{\theta}_i|\mathbf{Y})$ can be defined subjectively by the modeller (Beven and Binley, 1992). This allows for a likelihood function that does not necessarily reflect the parameter structure or model error variance (Stedinger et al., 2008). The choice of likelihood function can affect the accuracy of the estimated posterior distribution (He et al., 2010).

4.2.2.2. Markov Chain Monte Carlo

The MCMC approach approximates the posterior distribution by simulating a random walk that converges to the posterior probability distribution $P(\boldsymbol{\theta}|\mathbf{Y})$ that describes our updated beliefs of probable parameter values. A Markov chain is formed as each sequential approximate realisations from the distribution (from iteration $t = 1, \ldots, N$) is based on the previous draw. The MCMC process can be summarized as:

1. Define the Markov chain as $\boldsymbol{\Theta} = [\boldsymbol{\theta}_0, \ldots, \boldsymbol{\theta}_{t-1}, \boldsymbol{\theta}_t, \ldots, \boldsymbol{\theta}_N]$ for a chain of length N and select a starting parameter set $\boldsymbol{\theta}_0$.
2. Generate a candidate parameter set $\boldsymbol{\theta}_*$ based on a symmetric transition kernel $P(\boldsymbol{\theta}_*|\ \boldsymbol{\theta}_{t-1})$ such that: $P(\boldsymbol{\theta}_*|\ \boldsymbol{\theta}_{t-1}) = P(\boldsymbol{\theta}_{t-1}|\ \boldsymbol{\theta}_*)$.
3. Calculate the acceptance criteria (r) based on the ratio of densities (Metropolis et al., 1953) as:
$$r = \frac{P(\boldsymbol{\theta}_*|\mathbf{Y})}{P(\boldsymbol{\theta}_{t-1}|\mathbf{Y})} = \frac{P(\boldsymbol{\theta}_*)P(\mathbf{Y}|\boldsymbol{\theta}_*)}{P(\boldsymbol{\theta}_{t-1})P(\mathbf{Y}|\boldsymbol{\theta}_{t-1})} \tag{4.6}$$
4. If $\begin{cases} r > U[0,1] & \boldsymbol{\theta}_t = \boldsymbol{\theta}_* \\ r < U[0,1] & \boldsymbol{\theta}_t = \boldsymbol{\theta}_{t-1} \end{cases}$ where U[0,1] is a random draw from the uniform distribution between 0 and 1.

The Metropolis algorithm requires a symmetric transition kernel but can be generalized to the Metropolis-Hastings algorithm to allow for asymmetric transition kernels (Hastings, 1970; Gelman et al., 1997). In the above process, 2 to 4 are repeated for N iterations. A period of M iterations (referred to as the burn-in period) is required for the chain to converge to a stable posterior distribution. Therefore the remaining $n = N - M$ iterations represent draws from the posterior distribution. The total number of iterations required (N), the length of the burn-in period (M) and the transition kernel must be defined. The number of iterations must be long enough for the chain to converge. Convergence can be monitored by running several (J) consecutive chains from disparate starting parameter sets and computing the potential scale reduction statistic ($\sqrt{\hat{R}}$) (Gelman et al., 1997) as:

$$\sqrt{\hat{R}} = \sqrt{\frac{\frac{n-1}{n}W + \frac{1}{n}B}{W}} \tag{4.7}$$

for each parameter of interest. For a single parameter (θ), B is the between chain variance defined as:

$$B = \frac{n}{J-1}\sum_{j=1}^{J}(\bar{\theta}_{\cdot j} - \bar{\theta}_{\cdot\cdot})^2 \tag{4.7.1}$$

where

$$\bar{\theta}_{\cdot j} = \frac{1}{n}\sum_{i=1}^{n}\theta_{ij}$$

$$\bar{\theta}_{\cdot\cdot} = \frac{1}{J}\sum_{j=1}^{J}\bar{\theta}_{\cdot j}$$

and W is the within chain variance defined as:

$$W = \frac{1}{J}\sum_{j=1}^{J}s_j^2 \tag{4.7.2}$$

where

$$s_j^2 = \frac{1}{n-1}\sum_{i=1}^{n}(\theta_{ij} - \bar{\theta}_{\cdot j})^2.$$

Chains approach convergence as the variance between chains (4.7.1) approaches the variance within chains (4.7.2) based on the final n iterations from each of J chains. Gelman et al. (1997) recommend $\sqrt{\hat{R}}$ values of less than 1.2 are acceptable for most applications. For multi-dimensional problems convergence should be reached for all parameters. The posterior parameter distributions for each parameter can then be described using the posterior mean:

$$\hat{\mu}_{post} = \frac{1}{J \times n}\sum_{j=1}^{J}\sum_{i=1}^{n}\theta_{ij} \tag{4.8}$$

and variance:

$$\hat{\boldsymbol{\sigma}}_{post}^{2} = \frac{1}{(J \times n) - 1}\sum_{j=1}^{J}\sum_{i=1}^{n}(\theta_{ij} - \hat{\mu}_{post})^2 \tag{4.9}$$

of the n-by-J draws.

4.3. Materials and Methods

A dual approach was taken to evaluate the use of GLUE and MCMC as calibration tools for variety parameters in APSIM-Sugar. A theoretical and real world evaluation were performed. In the theoretical evaluation variety parameters were pre-defined for two varieties (V001 and

V002). GLUE and MCMC were then used to calibrate APSIM-Sugar using modified simulations of green biomass and sucrose yield as observed yields. This evaluated the ability of GLUE and MCMC calibrations to approach known parameter values. In the real world evaluation GLUE and MCMC were used to calibrate APSIM-Sugar for Australian variety Q117 based on observed green biomass and sucrose yields. The GLUE and MCMC estimated parameter values were validated using independent field trial data. This evaluated the ability of GLUE and MCMC calibrated parameter sets to produce simulated yields close to observed values. Uncertainty in model outputs due to uncertainty in the estimated parameter values was also analysed. A flow diagram of the methods used in this analysis is provided in Figure 4.2.

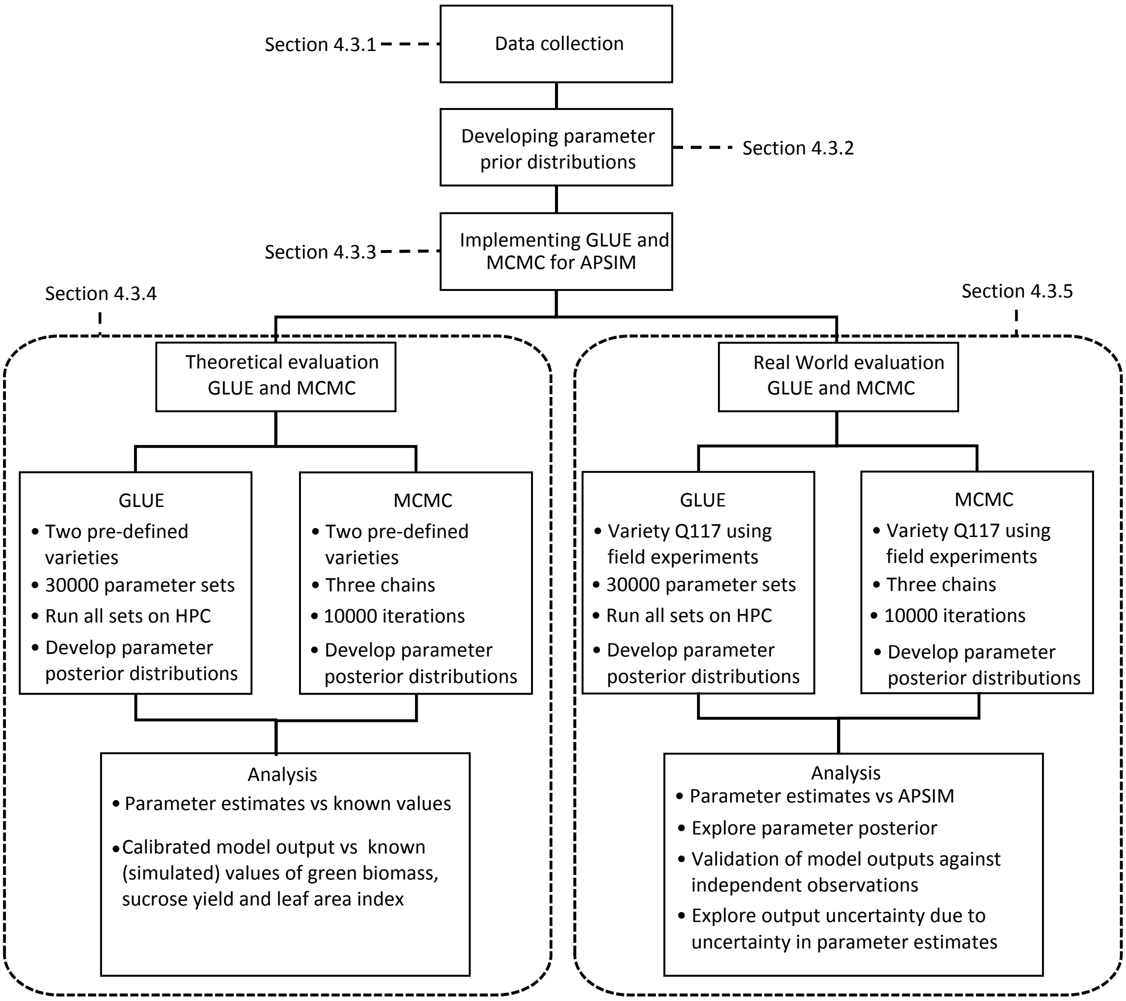

Figure 4.2. Diagrammatic representation of the materials and methods described in this chapter. Labels identify the relevant sections in the chapter. Section 4.3.1 to 4.3.3 describe general data collection and implementation of GLUE and MCMC for APSIM. Sections 4.3.4 and 4.3.5 detail the two approaches used to compare GLUE and MCMC. Theoretical evaluation allowed the comparison of estimated parameter values to explicitly known values while a real world application using field trial data allowed for the comparison of calibrated model outputs to real world data.

4.3.1. Data

Calibrations were performed using data from three field trials for variety Q117 run in Australia (Table 4.2). Each of the field experiments used for calibration were used in the development of APSIM-Sugar (Keating et al., 1999) and had the soil, climate and management data (e.g. irrigation and fertilizer applications) required to run APSIM simulations. Although other data sets exist, only APSIM-Sugar data sets for Q117 were considered in this study as the calibration for Q117 for APSIM was previously validated (Keating et al., 1999) providing a good comparison for the results of the two statistical calibration techniques used in this study.

The three field experiments were conducted at Harwood, New South Wales and Ingham, Queensland. The “Harwood(1993-94)” (Hughes et al., 1995) and “Ingham(1992-93)” (Robertson et al., 1996b) experiments were single 12 month plant crops well irrigated and fertilized to avoid stress. The “Ingham(1992-94)” experiment (Muchow et al., 1996a) had three nitrogen treatments. Crops in each treatment were harvested in 1993 and then ratooned (allowed to regrow) before being harvested again in 1994. The Harwood(1993-94) field experiment was characterised by cooler temperatures and lower levels of rainfall compared to the warmer and wetter Ingham field experiments (Table 4.2). Green biomass (g m^{-2}), sucrose yield (g m^{-2}) were sampled throughout the growing cycle for each treatment in the field experiments. From the three field experiments (Harwood(1993-94), Ingham(1992-93) and Ingham(1992-94)); eight yield samples were used as part of the calibration procedure (Harwood(1993-94), Ingham(1992-93), Ingham(1992-94) [low nitrogen; plant crop], Ingham(1992-94) [low nitrogen; ratoon crop], Ingham(1992-94) [med nitrogen; plant crop], Ingham(1992-94) [med nitrogen; ratoon crop], Ingham(1992-94) [high nitrogen; plant crop], Ingham(1992-94) [high nitrogen; ratoon crop]). The sample yields used for calibration were considered representative of harvest yields and the dates of these samples are recorded as ‘Harvest Date’ in Table 4.2.

Two additional field experiments were used as independent validations of GLUE and MCMC calibrations in the real world evaluation. These field experiments were conducted at Grafton, New South Wales (“Grafton(1994-95)”) and Ayr, Queensland (“Ayr(1994-95)”). These two field experiments were also used in the design of APSIM-Sugar (Keating et al., 1999). The Grafton(1994-95) field experiment was characterised by cooler conditions and higher rainfall than the Ayr(1992-94) experiment (Table 4.3). Both field experiments used for validation were well irrigated and fertilized to remove water and nutrient stresses. Green biomass, sucrose yield and LAI measurements for the validation experiments were taken 7 times during the

Grafton(1994-95) experiment and 24 times over the plant and first ratoon for the Ayr(1992-94) experiment. The date of the last sample is recorded as the 'Harvest Date' in Table 4.3.

Table 4.2. Details of field experiments used in both GLUE and MCMC calibrations of APSIM-Sugar. Average climate data were calculated as the average daily value for the period from planting to harvest.

	Harwood(1993-94)	**Ingham(1992-93)**	**Ingham(1992-94)**
Reference	(Hughes et al., 1995) [Dataset 1, Keating et al. (1999)]	(Robertson et al., 1996b) [Dataset 2, Keating et al. (1999)]	(Muchow et al., 1996a) [Dataset 16, Keating et al. (1999)]
Soil	PAWC = 180.0 mm	PAWC = 216.0 mm	PAWC = 216.0 mm
Avg. Min Temp.	18.11 ^{O}C	18.73 ^{O}C	18.80 ^{O}C
Avg. Max Temp.	24.67 ^{O}C	28.18 ^{O}C	28.39 ^{O}C
Avg. Daily Rainfall	1.86 mm	3.86 mm	4.44 mm
Plant Date	24-Sep-1993	23-Jul-1992	23-Jul-1992
Harvest Date	15-Dec-1994	14-Sep-1993	23-Aug-1994 (ratoon 16-Aug-1993)
Experiment Design	Plant crop; Fumigated	Plant crop; Fumigated	Plant crop and First ratoon; Fumigated Treatments: low, med and high Nitrogen

Table 4.3. Details of field experiments used for validation of both GLUE and MCMC calibrations of APSIM-Sugar. Average climate data is calculated as the daily average for the period from planting to harvest.

	Grafton(1994-95)	**Ayr(1992-94)**
Reference	[Dataset 11, Keating et al. (1999)]	[Dataset 6, Keating et al. (1999)]
Soil	PAWC = 180.0 mm	PAWC = 197.0 mm
Avg. Min Temp.	17.80 ^{O}C	21.05 ^{O}C
Avg. Max Temp.	25.96 ^{O}C	29.13 ^{O}C
Avg. Daily Rainfall	2.45 mm	1.01 mm
Plant Date	28-Sep-1994	31-Jul-1992
Harvest Date	25-Jul-1995	06-Sep-1994 (ratoon 29-Jul-1993)
Experiment Design	Plant crop; Fumigated	Plant crop and First ratoon; Non-Fumigated

4.3.2. Parameter prior distributions

Ten parameters were chosen for calibration based on the results from the global sensitivity analysis performed in Chapter 3. Of the 14 parameters the 10 parameters chosen for calibration were selected based on total sensitivity index scores for biomass and sucrose yield in Chapter 3. Table 4.4 lists the 10 parameters and their assumed prior distributions. Distributions used were the same as for Chapter 3 except for *green_leaf_no* and *rue* and k_L adjustment factors. The prior distribution of these parameters was based on observed data from a breeding trial study

(Basnayake et al. 2012b). To better reflect the distribution of parameter values estimated from the observed data, a normal distribution for *green_leaf_no*, *rue* and k_L was used. Data from an irrigated treatment grown at Home Hill, Queensland, Australia contained green leaf number measurements for 89 varieties. The distribution across the clones was approximately normal and the mean and standard deviation of the 89 varieties were used to describe a prior distribution for *green_leaf_no*. Similarly *rue* and k_L adjustment distributions (based on conductance measures as defined in Chapter 3) were found to be approximately normally distributed and the means and standard deviations of the 89 varieties were used to describe the prior distributions.

Table 4.4. Prior distributions assumed for statistical calibration of variety parameters. Uniform distributions were described as maximum and minimum allowed values. Normal distributions were described using mean and standard deviation (SD).

Parameter	Units	Distribution	Mean	SD	min	max
leaf_size (maximum)	mm^2	Uniform		-	20000	70000
cane_fraction	$g\ g^{-1}$	Uniform		-	0.65	0.80
sucrose_fraction_stalk	$g\ g^{-1}$	Uniform		-	0.4	0.7
sucrose_delay	$g\ m^2$	Uniform		-	0	600
min_sstem_sucrose	$g\ m^2$	Uniform		-	400	1500
tt_emerg_to_begcane	^oC day	Uniform		-	1200	2000
green_leaf_no	leaves	Normal	11.73	1.58	-	-
transp_eff_cf	$g\ kPa\ g^{-1}$	Uniform			0.0060	0.0140
rue adjustment factor[1]	nil	Normal	0.901	0.084	-	-
k_L adjustment factor[2]	nil	Normal	1.248	0.425	-	-

[1] an *rue* adjustment factor of 1 relates to the APSIM default rue of 1.8 g MJ^{-1} (plant) and 1.65 g MJ^{-1} (ratoon)

[2] a k_L adjustment factor of 1 relates to the default k_L based on APSIM Q117 and soil data.

4.3.3. Implementing GLUE and MCMC

Here, the computational process as well as the formulation of the transition kernel, likelihood and acceptance criteria is described. GLUE and MCMC were implemented within the R statistical program (R Core Team, 2013). Likelihoods and prior distributions were generated using the basic statistical package in R. Multivariate normal distributions were generated using the MASS package (Venables and Ripley, 2002). The APSIMBatch (Zheng, 2012) package 'generateSim' function was modified to generate the simulation files needed to run APSIM-Sugar. The functions written in the R environment to run GLUE and MCMC were compiled into an R package called Bayes4APSIM (available on request).

Both GLUE and MCMC calibrations were based on the field experiments described in Table 4.2. Model errors were assumed normally distributed and a normal likelihood function (4.10) was used. The Likelihood value for each parameter set was calculated based on observed green biomass and sucrose yields at harvest. Error variance was estimated for harvest green biomass ($\sigma^2_{\text{biomass}}$) and sucrose yield ($\sigma^2_{\text{sucrose}}$) but not for individual experiments. These variances were then fixed (assumed known, with no uncertainty). To avoid problems with computer precision within R likelihoods

$$L(\boldsymbol{\theta}_i \mid \mathbf{Y}) = \prod_{s=1}^{S}\prod_{o=1}^{O} \frac{1}{\sqrt{2\pi\sigma_s^{2}}} \exp\left(-\frac{[y_{os} - \hat{y}_{os}(\boldsymbol{\theta}_i)]^2}{2\sigma_s^{2}} \right) \tag{4.10}$$

were calculated as log-likelihoods

$$\ln[L(\boldsymbol{\theta}_i \mid \mathbf{Y})] = -\frac{O \times S}{2} \cdot \ln(2\pi) - \frac{O}{2}\sum_{s=1}^{S} \ln(\sigma_s^{2}) - \frac{1}{2}\sum_{s=1}^{S}\sum_{o=1}^{O} \frac{[y_{os} - \hat{y}_{os}(\boldsymbol{\theta}_i)]^2}{\sigma_s^{2}} . \tag{4.11}$$

Here S is the number of productivity measures considered (S = 2), specifically green biomass and sucrose yield and O is the number of observations of each measure (O = 8), specifically harvest yields from experiments Harwood(1993-94), Ingham(1992-93), Ingham(1992-94) (low, med and high nitrogen; plant and first ratoon).

4.3.3.1. Implementing GLUE

Prior distributions were used to generate 30000 (Q) parameter sets. Parameter sets were then run simultaneously on a high performance cluster. Harvest green biomass and sucrose yield were simulated to match the scenarios of the calibration field experiments (Table 4.2). Log-likelihoods were calculated for all parameter sets using (4.11). The equation for GLUE posterior probabilities (4.3) was modified to use log-likelihoods and posterior probabilities were calculated as

$$p(\boldsymbol{\theta}_i) = \frac{L(\boldsymbol{\theta}_i \mid \mathbf{Y})}{\sum_{i=1}^{Q} L(\boldsymbol{\theta}_i \mid \mathbf{Y})} = \frac{\exp(\ln[L(\boldsymbol{\theta}_i \mid \mathbf{Y})])}{\sum_{i=1}^{Q} \exp(\ln[L(\boldsymbol{\theta}_i \mid \mathbf{Y})])} . \tag{4.12}$$

The posterior distribution for each parameter was defined by the posterior mean (4.4) and variance (4.5). A diagrammatic representation of the GLUE process is presented in Figure 4.3.

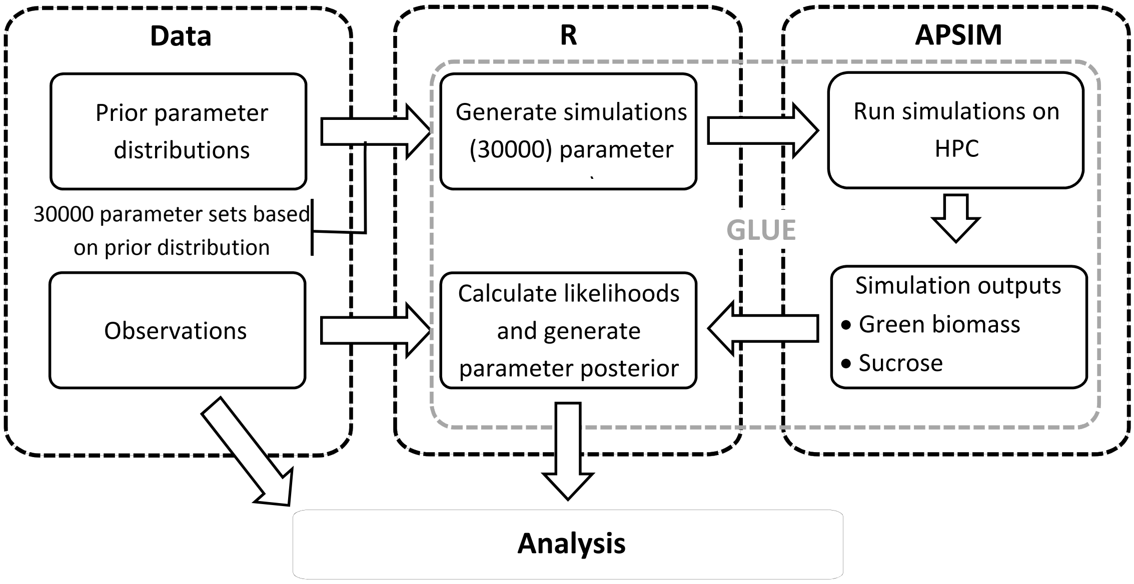

Figure 4.3. Diagrammatic representation of the application of GLUE to APSIM used in this study. Prior parameter distributions were used to generate 30000 parameter sets. These were run on a HPC cluster for efficiency. Likelihood values were calculated for all 30000 sets and final posterior parameter distributions were developed for each parameter.

4.3.3.2. Implementing MCMC

For implementation of MCMC it is simpler to consider a single chain. For each chain, a candidate parameter set ($\boldsymbol{\theta}_*$) was generated from the multivariate normal distribution ($\boldsymbol{\theta}_*|\boldsymbol{\theta}_{t-1} \sim N(\boldsymbol{\theta}_{t-1}, k\boldsymbol{\Sigma})$). Parameters were assumed independent such that the covariance matrix ($\boldsymbol{\Sigma}$) was diagonal with variances derived from the prior distributions. The covariance matrix was modified by k = 0.01 as this was found using a grid based optimization search to produce an acceptance rate between 30 and 40 percent (Gelman et al., 1997). As log-likelihoods were calculated, the acceptance criterion (4.6) was calculated using log-likelihoods as

$$r = \frac{P(\boldsymbol{\theta}_*)L(\boldsymbol{\theta}_*|\mathbf{Y})}{P(\boldsymbol{\theta}_{t\text{-}1})L(\boldsymbol{\theta}_{t\text{-}1}|\mathbf{Y})} = \exp((\ln[P(\boldsymbol{\theta}_*)] + \ln[L(\boldsymbol{\theta}_*|\mathbf{Y})]) - (\ln[P(\boldsymbol{\theta}_{t\text{-}1})] + \ln[L(\boldsymbol{\theta}_{t\text{-}1}|\mathbf{Y})])) \,. \qquad (4.13)$$

Chains were set to a length of 10000 iterations (N). Three simultaneous chains (J = 3) were run to monitor convergence of the posterior distribution. Following (4.8) and (4.9), posterior means and variances were calculated as the final 5000 (M) iterations of each chain. Posterior distributions were generated on samples of 15000 (n) parameter sets. A diagrammatic representation of the MCMC process is presented in Figure 4.4.

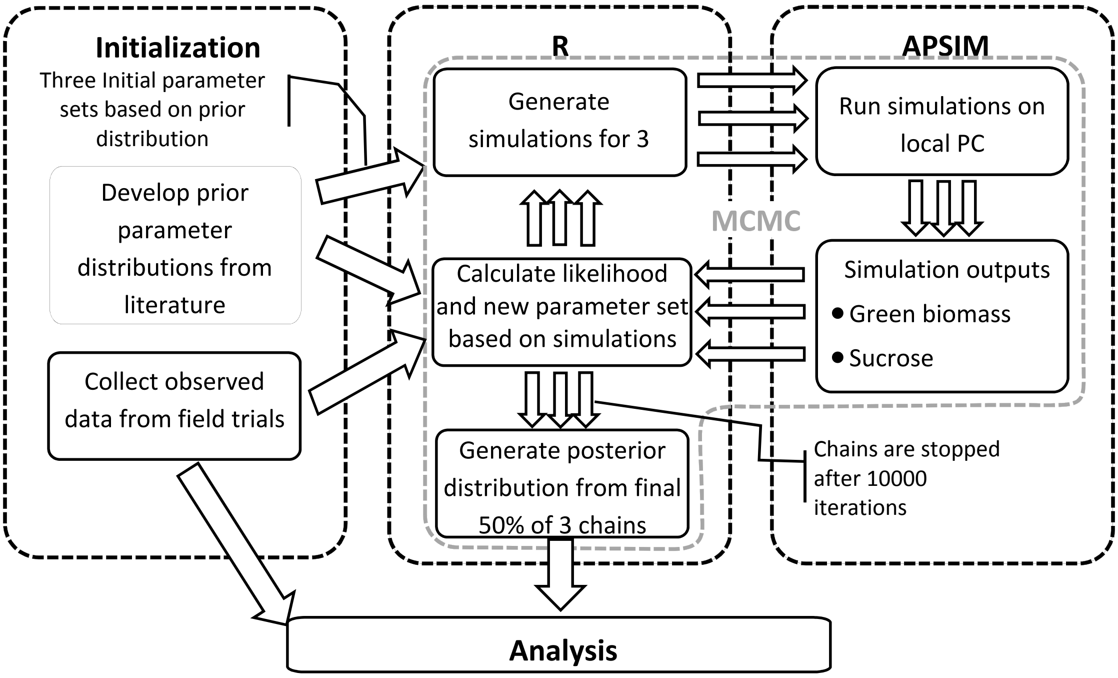

Figure 4.4. Diagrammatic representation of the application of MCMC to APSIM used in this chapter. Prior parameter distributions were used to generate three initial parameter sets. These initial parameter sets were used to generate three chains from 10000 iterations. Convergence of the three chains to a single posterior distribution was monitored and the final posterior parameter distribution was developed from the final 50% of all chains.

4.3.4. Theoretical evaluation of GLUE and MCMC

Two varieties referred to as V001 and V002 were pre-defined using 10 influential parameters (Table 4.5). The leaf size parameter (*leaf_size*) for V001 was made larger than typically seen in Australian field experiments while parameters *cane_fraction*, *min_sstem_sucrose* and *sucrose_delay* were set to lower values to increase sucrose and cane yields. Sucrose fraction was raised higher to increase sucrose yields. Variety V002 represented a smaller plant with a lower sucrose yield. Parameters representing the transpiration efficiency coefficient (*transp_eff_cf*), RUE (*rue*) and root conductance (k_L) were higher in V002 than V001. An increased *transp_eff_cf* and increased k_L can improve performance in water stressed conditions (Inman-Bamber et al., 2012).

Table 4.5. Parameter values for two pre-defined varieties V001 and V002. The parameter *leaf_size* is expressed as leaf size for each leaf number modelled on variety Q117. Parameters *rue* and k_L were modified relative to the default simulation values used in Keating et al. (1999) for variety Q117 and are represented here as a unitless fraction of the original value. All other parameters appear as the values required by APSIM-Sugar.

Parameter	Units	V001			V002		
leaf_size	mm^2	1718.182	63000	63000	954.546	35000	35000
leaf_size_no	leaf	1	14	20	1	14	20
cane_fraction	g g^{-1}			0.66			0.74
sucrose_fraction_stalk	g g^{-1}			0.65			0.46
sucrose_delay	g m^{-2}			100			400
min_sstem_sucrose	g m^{-2}			550			1000
tt_emerg_to_begcane	°C d			1500			1860
green_leaf_no	leaves			14			11
transp_eff_cf	kPa			0.0087			0.0100
rue adjustment factor	nil			0.89^1			1.02^1
k_L adjustment factor	nil			0.60^2			1.20^2

^{1} adjustment factors resulted in an actual rue of 1.602 (plant) and 1.469 (ratoon) for V001 and 1.836 (plant) and 1.02 (ratoon) for V002

^{2} adjustment factors resulted in an actual k_L of 0.096 and 0.192 for V001 and V002 respectively

APSIM was used to produce simulated yields ($\hat{y}_i(\theta_j)$) for the pre-defined varieties V001 and V002 for calibration field experiments (Table 4.2). To represent realistic uncertainty in data collection, a normal error was added to simulated yields to generate 'observed' yields (o_{ij}) for varieties V001 and V002. Error was added as a random number drawn from a normal distribution with zero mean and standard deviation (SD) of 5% of simulated yield. This represented the increasing uncertainty in field measurements as values increased and allowed variance to be smaller early in the season or where limiting factors may have reduced yields and yield variances. Both GLUE and MCMC error variances for green biomass and sucrose yield were set to the variance used to generate the observed data (i.e. 5% of yield).

Both GLUE and MCMC were used to estimate the 10 variety parameters for V001 and V002. Posterior distributions for each parameter were recorded. The absolute relative error (ARE)

$$ARE = \frac{|\overline{\theta}_{post} - \theta_0|}{\theta_0} \times 100 \tag{4.14}$$

was calculated between the posterior mean and known value for each parameter of the defined varieties (Table 4.5). The fit between calibrated simulation outputs and observed data was assessed using normalized root mean square error (NRMSE), Willmott's agreement index (D) (Willmott, 1982; Marin et al., 2011) and regression r^2. The slope and intercept of the linear regression between calibrated simulation outputs and observations were also recorded. Statistical analysis was performed on green biomass (g m^{-2}) and sucrose yield (g m^{-2}). Root mean square error was normalized and expressed as a percentage by dividing by the range of observed values. This allowed comparison between model outputs.

4.3.5. Real world evaluation of GLUE and MCMC for variety Q117

Observed harvest yields for Q117 for the calibration experiments (Table 4.2) were used to estimate the 10 variety parameters for Q117. Standard deviations for the likelihood function were based on the error variance of a simulation using default parameter values for variety Q117. As with the theoretical evaluation, posterior distributions were generated. Calibrated parameter values were compared to the default values for Q117 contained in APSIM-Sugar, using the absolute relative error (ARE). GLUE and MCMC parameter estimates were used to simulate sugarcane yields for two independent validation field trials (Table 4.3). As several measurements were made throughout the validation trials, the observed growth curves were simulated. Regression statistics (slope, intercept and r^2), D and NRMSE were calculated for each experiment using all available data and data at harvest only. Uncertainty in model outputs for green biomass, sucrose yield and LAI were investigated by producing 95% credible intervals from 1000 random draws of the parameter posterior distributions.

4.4. Results and Discussion

4.4.1. Theoretical evaluation of GLUE and MCMC

This chapter evaluated the use of GLUE and MCMC to calibrate the APSIM-Sugar model for two pre-defined sugarcane varieties. Both GLUE and MCMC were able to accurately estimate known variety parameters (Table 4.6). Standard deviations for each parameter posterior distributions were recorded to identify uncertainty in the parameter estimates. For both pre-defined varieties 60% of GLUE parameter estimates and 70% of MCMC parameter estimates were within 10% of the defined values. Importantly estimated parameter values differed accurately between variety V001 and V002. For example *transp_eff_cf*, *rue* and k_L were particularly well estimated for V001 and V002 using the MCMC calibration resulting in realistic differences in these parameters between the two varieties. These parameters in particular may play an important role in improving differences in response to water stress between sugarcane varieties (Inman-Bamber et al., 2012) but are difficult to measure directly. Therefore it is a critical result that these parameters can be accurately estimated using only harvest data.

Table 4.6. GLUE and MCMC evaluation of estimated parameter values for two pre-defined varieties (V001 and V002). Mean and standard deviation of the empirical posterior distributions are recorded. The ARE measures the absolute difference between the posterior mean and the defined value as a percentage. For MCMC all chains were assumed to converge for all parameters as $\sqrt{\hat{R}}$ was less than 1.2 for all parameters.

Variety	Parameter	Value	GLUE		MCMC	
			Mean (SD)	**ARE**	**Mean (SD)**	**ARE**
V001	*leaf_size*	63000	56065.03(3181.31)	11.0	56630.50(7956.9)	10.1
	cane_fraction	0.66	0.665(0.021)	0.8	0.671(0.0159)	1.7
	sucrose_fraction_stalk	0.65	0.666(0.014)	2.5	0.621(0.0413)	4.5
	sucrose_delay	100	373.96(94.91)	274.0	305.56(154.10)	205.6
	min_sstem_sucrose	550	661.98(100.54)	20.4	700.13(161.25)	27.3
	tt_emerg_to_begcane	1500	1461.19(95.37)	2.6	1445.03(136.57)	3.7
	green_leaf_no	14	12.37(0.441)	11.7	13.04(0.801)	6.8
	transp_eff_cf	0.0078	0.0077(0.0003)	1.9	0.0078(0.0004)	0.4
	rue adjustment factor	0.89	0.942(0.012)	5.8	0.934(0.035)	4.9
	k_L adjustment factor	0.60	0.548(0.039)	8.6	0.577(0.085)	3.9
			Average ARE (%)	33.9	**Average ARE (%)**	26.9
V002	*leaf_size*	35000	27952.67(5592.94)	20.1	34289.87(4928.9)	2.0
	cane_fraction	0.74	0.780(0.031)	5.4	0.710(0.029)	4.0
	sucrose_fraction_stalk	0.46	0.473(0.015)	2.8	0.469(0.029)	2.1
	sucrose_delay	400	416.02(63.78)	4.0	507.99(71.02)	27.0
	min_sstem_sucrose	1000	995.04(94.85)	0.5	799.52(232.20)	20.1
	tt_emerg_to_begcane	1860	1876.21(73.87)	0.9	1834.42(101.85)	1.4
	green_leaf_no	11	10.38(0.765)	5.6	11.25(0.712)	2.2
	transp_eff_cf	0.011	0.0126(0.00083)	15.0	0.0124(0.00102)	12.6
	rue adjustment factor	1.02	1.14(0.072)	12.3	1.014(0.046)	0.5
	k_L adjustment factor	1.20	1.32 (0.244)	10.2	1.138(0.35)	5.2
			Average ARE (%)	7.7	**Average ARE (%)**	7.7

The parameter *sucrose_delay* was particularly poorly estimated for V001 using both GLUE and MCMC. This may have been a consequence of weak influence of the parameter on sucrose yield. Chapter 3 showed that *sucrose_delay* was weakly influential for sucrose under both irrigated and water stressed conditions. Particularly *sucrose_delay* had less influence on sucrose yields at low values (Figure 3.2 (d)). This may explain why *sucrose_delay* estimates for V002 were much closer than for V001. Similarly *leaf_size* and *transp_eff_cf* estimates were closer when known values were low and high respectively, reflecting regions where these parameter values had a greater influence on yields. Several recent studies have used techniques such as GLUE and MCMC to calibrate crop models for varieties based on observed yields.

Figure 4.5 shows the linear regression between the APSIM generated and calibrated APSIM simulated green biomass and sucrose yield values for V001 and V002. As would be expected from the accurate estimation of parameter values, both GLUE and MCMC calibrations accurately reproduced the APSIM generated biomass and sucrose yields used in the model calibration. For both pre-defined varieties, both GLUE and MCMC calibrated simulations of green biomass were closer to the calibration data than sucrose yield based on NRMSE. This was likely a consequence of the poorer estimation of sucrose parameters. The real world evaluation provided a better indication of GLUE and MCMC to replicate observed yields using independent validation datasets.

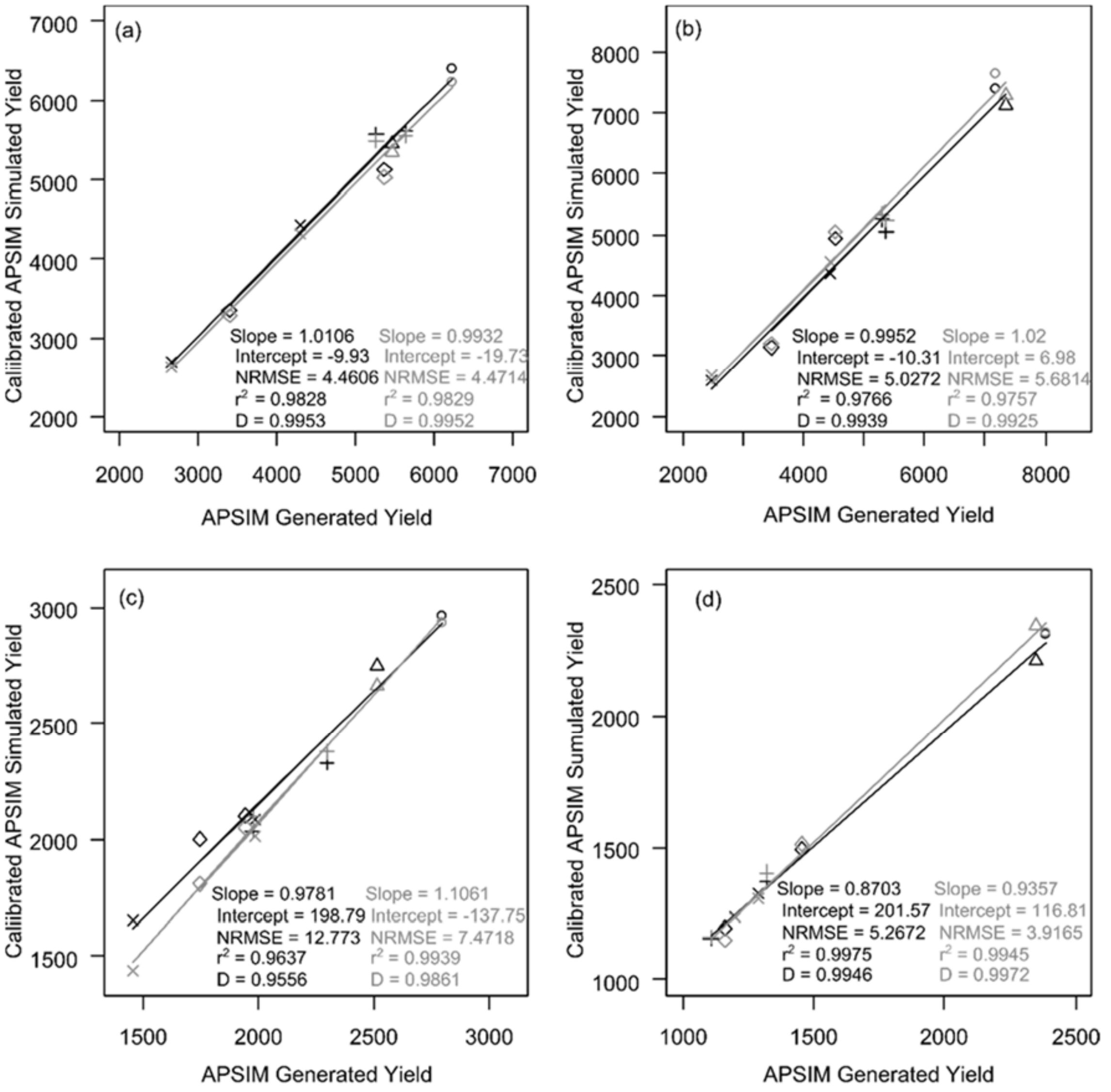

Figure 4.5. Linear regression between APSIM generated yields used in the calibration and calibrated APSIM simulated values for (a, b) green biomass (g m^{-2}) and (c, d) sucrose yield (g m^{-2}) for pre-defined varieties V001 (a, c) and V002 (b, d). Results from MCMC (black) and GLUE (grey) are plotted. Data represent simulations of V001 and V002 for Harwood(1993-94) (○), Ingham(1992-93) (△), Ingham(1992-94) low Nitrogen (✕), Ingham(1992-94) med Nitrogen (◇) and Ingham(1992-94) high Nitrogen (+) trials.

4.4.2. Real world evaluation of GLUE and MCMC for Variety Q117

Estimated parameter values using GLUE were closer to APSIM-Sugar default values for variety Q117 (Table 4.7). Compared to APSIM-Sugar default values GLUE estimated a higher *leaf_size* and low *min_sstem_sucrose* while MCMC estimated a lower *leaf_size* and *tt_emerg_to_begcane* and a higher *green_leaf_no*. Both GLUE and MCMC estimated values for *sucrose_delay* differed greatly from default values. As with the theoretical evaluation this was likely a consequence of the low influence of *sucrose_delay* on simulated yields. Similarly GLUE and MCMC estimates of k_L varied greatly with the expected default value. Although this was not an issue in the theoretical evaluation, it may be that a weak influence on yields complicated the estimation techniques. Both k_L and *sucrose_delay* had total sensitivity index values of < 5% under irrigated or stressed conditions (Chapter 3).

Table 4.7. GLUE and MCMC comparison of estimating correct parameter values for Q117. Mean and standard deviation of the empirical posterior distributions are recorded. For MCMC all chains converge for all parameters ($\sqrt{\hat{R}} < 1.2$) except *sucrose_delay* ($\sqrt{\hat{R}} > 1.2$).

Parameter	**Q117**	**GLUE** **Mean (SD)**	**MCMC** **Mean (SD)**
leaf_size	55000	61971.11(6704.96)	39921.81(3665.07)
cane_fraction	0.70	0.730(0.010)	0.670(0.0216)
sucrose_fraction_stalk	0.55	0.581(0.025)	0.553(0.0596)
sucrose_delay	0	133.82(84.36)	253.20(101.94)
min_sstem_sucrose	800	589.56(283.28)	1253.56(165.95)
tt_emerg_to_begcane	1900	1853.37(199.81)	1396.49(131.89)
green_leaf_no	13	13.97(0.343)	16.38(0.916)
transp_eff_cf	0.0080	0.0081(0.00051)	0.00890(0.00055)
rue adjustment factor	1	1.030(0.019)	1.033(0.0314)
k_L adjustment factor	1	0.367 (0.026)	0.266(0.0349)

In contrast to k_L, *rue* and *transp_eff_cf* parameters agreed closely with expected (default) values. Radiation use efficiency is a difficult trait to measure and the *rue* parameter in APSIM greatly influences model outputs. The agreement between *transp_eff_cf* and default values is especially encouraging given the wide prior distribution. The default value for *transp_eff_cf* was based on literature for other C_4 crops such as sorghum which have a value of 0.009 g kPa g^{-1} (Keating et al., 1999; Sinclair, 2012). Inman-Bamber and McGlinchey (2003) derived a *transp_eff_cf* of 0.0087 g kPa g^{-1} for variety Q138. The MCMC and GLUE estimates while based on only a small sample of sites, closely aligns with this recorded value and provides a measure of uncertainty not available with the original calibration. The lower *leaf_size* value of the MCMC calibration may more closely represent field measured values than the higher GLUE estimate. While maximum leaf area has been measured as high as 70000 mm^2 under high input glasshouse studies (Inman-Bamber, 2013), under field conditions values of 38000 mm^2 were more common (Robertson et al., 1998). This would seem a more realistic calibrated value based on field measures of yield.

To further explore uncertainty in parameter posterior uncertainty, posterior probability distributions were analysed. Parameter uncertainty was lower for GLUE parameter posterior distributions based on standard deviations for all parameters except *leaf_size*, *min_sstem_sucrose* and *tt_emerg_to_begcane* (Table 4.7). However, the empirical posterior distribution did not always follow a normal distribution as assumed. Figure 4.6 shows, as an example, the posterior distribution of *tt_emerg_to_begcane* for GLUE and MCMC calibrations. The GLUE empirical distribution of *tt_emerg_to_begcane* had a distinct major and minor mode while the MCMC empirical distribution of *tt_emerge_to_begcane* was biased towards lower values. While multimodal posterior distributions are not uncommon, these results suggests that the mean of the posterior distribution may not be the most ideal parameter set to use as calibrated parameter values.

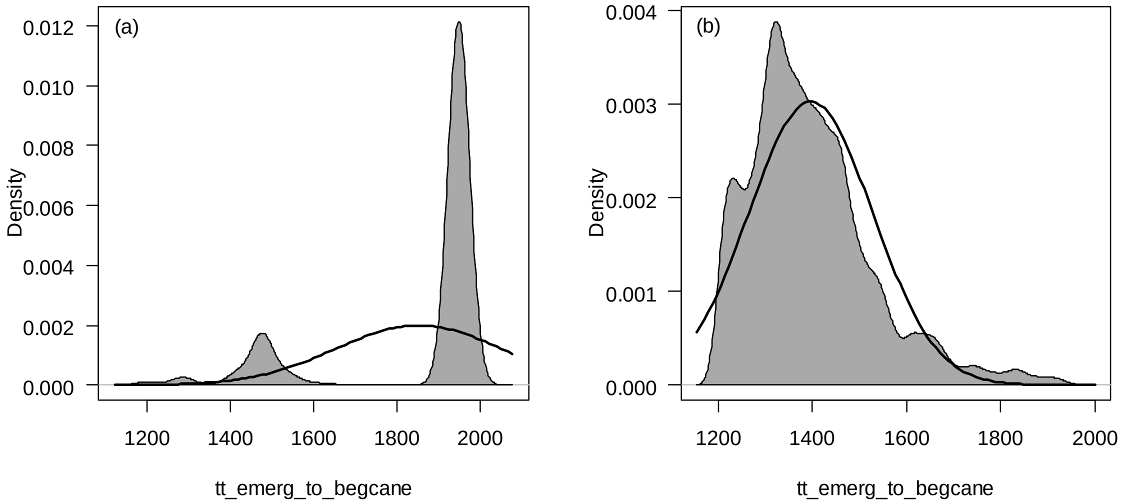

Figure 4.6. Empirical posterior probability density functions (grey) for parameter *tt_emerge_to_begcane* (°C d) and approximate normal distribution (—) based on the mean and standard deviations reported in Table 4.7 for (a) GLUE and (b) MCMC.

Based on all available samples from two validation experiments both GLUE and MCMC calibrations produced lower NRMSE and higher r^2 values for green biomass and sucrose yield model outputs compared to default APSIM values for Q117 (Table 4.8). Green biomass was the most accurately simulated output in all cases while simulated LAI had the highest NRMSE and lowest r^2 and D values of the three outputs analysed. This agrees with results from the original model validation (Keating et al., 1999). Simulation of LAI may have been improved if LAI had been used in the model calibration but is rarely measured in field experiments. Based on NRMSE and D index, green biomass, sucrose yield and LAI simulations were slightly better using the MCMC calibration compared to the GLUE calibration.

Table 4.8. Comparison of simulated to observed green biomass, sucrose yield and LAI using APSIM-Sugar default parameter values for Q117, GLUE and MCMC calibration posterior means. NRMSE was calculated as the root mean square error divided by the output range expressed as a percentage. The r^2 was calculated from the linear regression between observed and simulated values. Willmott's agreement index (D) is a non-parametric goodness-of-fit measure, similarly to r^2 a value close to one is desired.

Output	Experiment	N	APSIM Q117 Default			MCMC			GLUE		
			NRMSE	r^2	D	NRMSE	r^2	D	NRMSE	r^2	D
Green Biomass	Grafton(1994-95)	7	7.61	0.99	0.99	7.13	0.98	0.99	4.83	0.98	1.00
	Ayr(1992-94)	24	16.11	0.80	0.95	9.24	0.93	0.98	12.37	0.88	0.97
	Harvest	3	22.58	0.85	0.94	8.37	0.99	0.99	15.65	0.95	0.97
	All Data	31	14.28	0.83	0.95	8.30	0.94	0.98	10.94	0.89	0.97
Sucrose yield	Grafton(1994-95)	4	20.11	0.99	0.94	19.37	0.98	0.95	21.84	0.99	0.94
	Ayr(1992-94)	17	16.64	0.77	0.93	13.97	0.84	0.98	16.87	0.87	0.94
	Harvest	3	16.88	0.99	0.97	17.76	0.99	0.96	23.93	1.00	0.94
	All Data	21	15.14	0.81	0.95	12.76	0.88	0.96	15.38	0.89	0.95
LAI	Grafton(1994-95)	7	11.03	0.94	0.98	16.95	0.86	0.95	15.13	0.92	0.97
	Ayr(1992-94)	24	17.42	0.70	0.90	15.75	0.85	0.91	16.47	0.70	0.91
	Harvest	3	13.23	0.99	0.97	11.03	1.00	0.98	10.92	0.98	0.99
	All Data	31	14.84	0.78	0.93	14.92	0.85	0.93	14.97	0.78	0.94

Despite both calibrations having high r^2 and D values, simulated outputs could differ noticeably (Figure 4.7). The high simulated LAI using GLUE parameter estimates is likely a result of the high value of *leaf_size*. Figure 4.8 shows the time course of observations and simulated values using both GLUE and MCMC calibrations (solid lines) as well as a 95% credible interval based on 1000 random draws from the posterior distributions (dashed lines). The solid grey line of Figure 4.8 (c) shows that this high *leaf_size* helped simulate peak values of LAI in the Grafton(1994-95) experiment but likely also lead to overestimating lower values of LAI. Conversely, simulated LAI using MCMC parameter estimates underestimated peak LAI in the Grafton(1994-95) experiment but accurately estimated lower value (Figure 4.8 (c) solid black line). The different parameter estimates of GLUE and MCMC lead to similar simulated green biomass and sucrose yield accumulation curves. However, the difference in parameter uncertainty lead to very different uncertainty in simulated sucrose yield (Figure 4.8 (b)). The wide 95% credible interval for sucrose yield based on the GLUE posterior distribution is likely a result of the higher uncertainty in *min_sstem_sucrose* and *tt_emerge_to_begcane* parameters which determines when sucrose accumulation starts. The large difference in output uncertainty due to parameter uncertainty between the GLUE and MCMC calibrations highlights the importance of reporting the uncertainty along with estimated parameter values when using statistical calibration techniques.

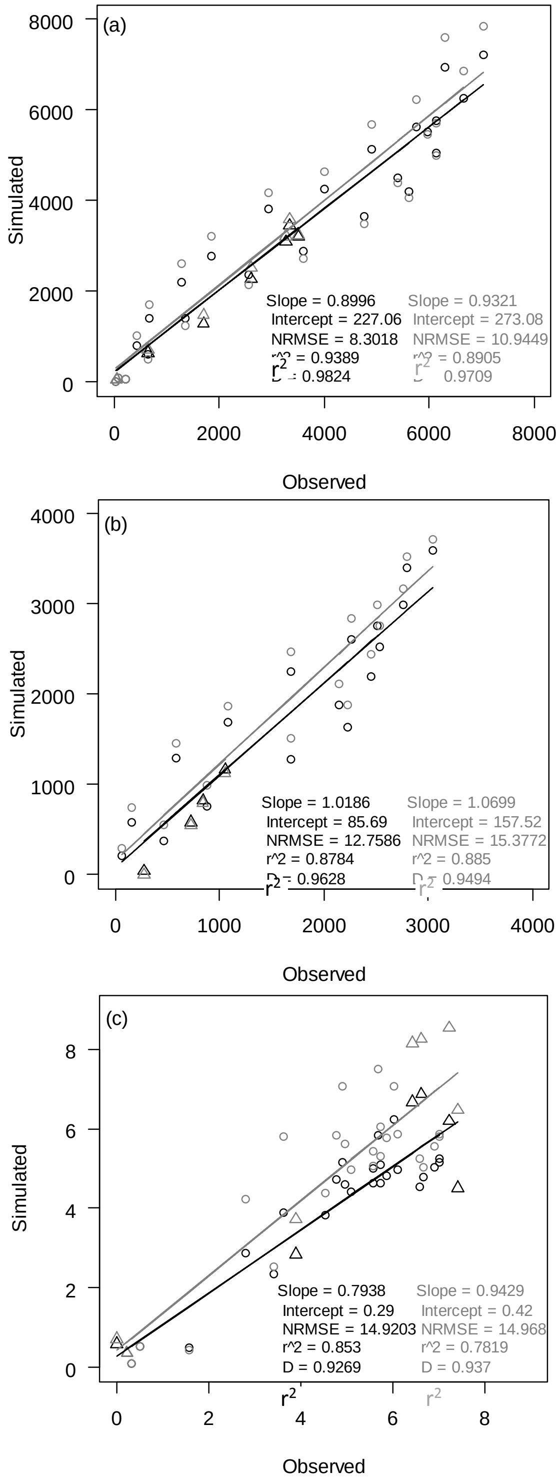

Figure 4.7. Linear regression between observed and simulated (a) green biomass (g m^{-2}), (b) sucrose yield (g m^{-2}) and (c) leaf area index for Q117. Results from GLUE (—) and MCMC (—) are plotted across all samples taken from Grafton(1994-95) (△) and Ayr(1992-94) (○) validation experiments.

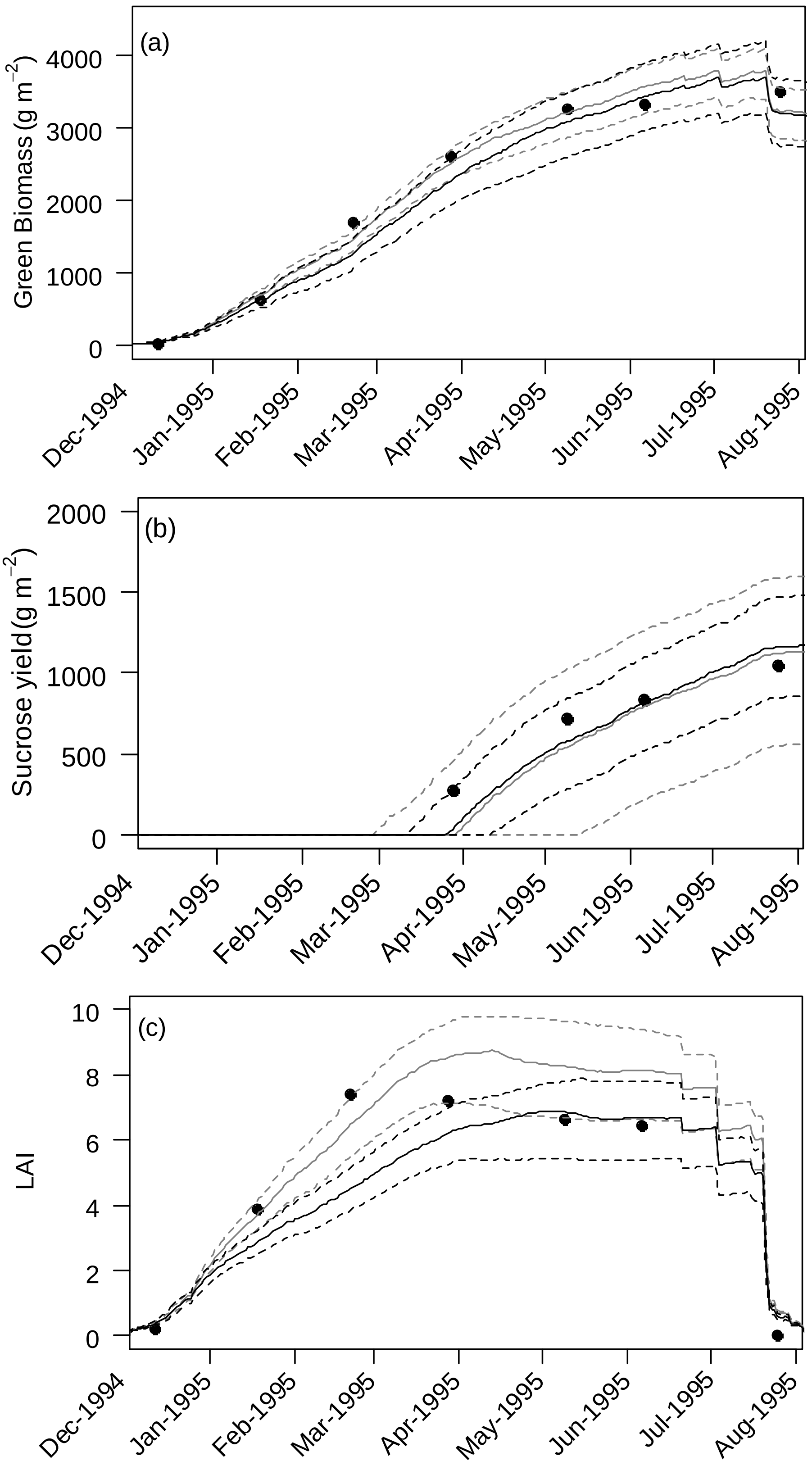

Figure 4.8. Time series comparison of simulated and observed values (•) for Q117 in Grafton(1994-95). (a) green biomass (b) sucrose yield and (c) leaf area index (LAI). Solid lines represent simulated values using parameter posterior means for GLUE (—) and MCMC (—). Dashed lines represent a 95% confidence interal based on 1000 random draws from the parameter posterior distributions

4.5. Conclusions and Recommendations

This chapter evaluated the use of GLUE and MCMC as techniques for calibrating APSIM-Sugar for different sugarcane varieties. Both GLUE and MCMC calibrations were able to accurately simulate green biomass and sucrose yield in both a theoretical and real world evaluation. In fact based on NRMSE, r^2 and D statistics, there was little difference in the accuracy of GLUE and MCMC. The evaluation of GLUE and MCMC was extended by using two pre-defined varieties in the theoretical evaluation. Both GLUE and MCMC were able to estimate the differences in parameter values between the two pre-defined varieties. This kind of analysis has not been performed before for a sugarcane model and strongly supports the use of statistical calibration techniques in calibrating APSIM-Sugar for different varieties.

Although there was little difference in the skill of GLUE and MCMC in either the theoretical or real world evaluation, I recommend modellers consider the use of MCMC in calibrating variety parameters in sugarcane models. MCMC produced slightly lower ARE between estimated and pre-defined parameter values than GLUE in the theoretical evaluation. MCMC also produced improved validation NRMSE and r^2 for observed green biomass and sucrose yield in the real world evaluation. The inclusion of multiple chains in MCMC provided an objective method for assessing the convergence and stability of the posterior distribution of the variety parameters.

There are several opportunities to improve either estimation technique. The main limitation of this research was the use of simplistic GLUE and MCMC algorithms. I recommend that modellers in future apply more advanced adaptive MCMC algorithms. This could include extending calibration data sets to include measurements made throughout the season and better reflecting the structure of the error variance by use of an appropriate transformation of the likelihood function, similar to the work of Dumont et al. (2014). Calibration efficiency could also be improved by including covariance between variables. Where these are not known, preliminary MCMC runs could be used to estimate the structure of parameter covariance.

A further limitation identified in both the theoretical and real world evaluation was the inclusion of parameters with relatively weak influence on the outputs used in calibration. The *sucrose_delay* parameter was particularly poorly estimated in the theoretical evaluation while the estimated value of k_L in the real world evaluation could not be easily explained physiologically. Future research may need to avoid using these parameters in calibration. The difficulties that arose in estimating the *sucrose_delay* and k_L parameter values also highlights the need for future calibration methods to more formally consider the different sources of model error as described by Kennedy and O'Hagan (2001). Unusual or unexpected parameter values from calibrations may reflect some form of model limitation and may be used to identify a source of error in the specific simulation or highlight an area in the model where further research in the underlying physiology could be explored.

Finally, it is important to acknowledge that the GLUE and MCMC calibrations in this chapter were performed on a subset of the data sets used in the original model validation. Therefore the purpose of this chapter however, was not to supply an updated calibration of APSIM-Sugar for variety Q117 but to evaluate the use of statistical calibration of variety parameters. Parameters that are difficult to measure can be estimated using a limited amount of data such as biomass and sucrose yields which are routinely collected in breeding programs. Statistical calibration techniques such as MCMC should be used to update APSIM-Sugar as varieties are developed. With appropriate variety definitions, APSIM-Sugar could be used for early risk assessment of adopting new varieties in different growing environments.

4.6. Chapter 4 Summary

Process-based agricultural systems models allow researchers to investigate the interactions between variety, environment and management. The 'Sugar' module in the Agricultural Production Systems sIMulator (APSIM-Sugar) currently includes definitions for 14 sugarcane varieties, most of which are no longer commercially grown. The use of two Bayesian approaches to calibrate sugarcane varieties in APSIM-Sugar: Generalized Likelihood Uncertainty Estimation (GLUE) and Markov Chain Monte Carlo (MCMC) was evaluated in this chapter. Both GLUE and MCMC calibrations were able to accurately simulate green biomass and sucrose yield in both a theoretical and real world evaluation. In a theoretical evaluation GLUE and MCMC parameter estimates accurately reflected differences between two pre-defined sugarcane varieties. MCMC was capable of more in-depth analysis of calibrated parameter uncertainty. Calibration techniques such as MCMC can be used to calibrate varieties in APSIM-Sugar based on yield data. With appropriate variety definitions, APSIM-Sugar could be used for early risk assessment of adopting new varieties.

Chapter 5

Thesis Conclusion

Process-based agricultural production systems simulators allow researchers to investigate the interactions between crop varieties, growing environments and management practices without having to conduct laborious, expensive field trials that can run for several years. These interactions have been investigated by modifying variety parameters in crop models for many different crops. However, similar simulation studies for sugarcane are rare in the current literature (Chapter 1). Moreover, current leading sugarcane models do not reflect the range of sugarcane varieties currently grown for commercial yields (Chapter 4). By better understanding how sugarcane crop models represent different varieties through variety parameters and developing the tools necessary to update these representations, the use of sugarcane crop models as decision support tools can be improved.

A review of the literature (Chapter 1) highlighted that statistical tools such as sensitivity analysis and statistical calibration that have been used for other crops to advance variety modelling have not been widely explored for sugarcane. This thesis made a significant contribution towards advancing the simulation of varietal difference using the 'Sugar' module in the Agricultural Production Systems sIMulator (APSIM-Sugar) by:

1. Investigating the capability of the APSIM-Sugar model to simulate yield differences between sugarcane varieties under different climatic conditions (Chapter 2);
2. Investigating the influence of variety parameters on key model outputs using statistical sensitivity analysis (Chapter 3) and
3. evaluating the use of two Bayesian approaches to statistically calibrate variety parameters in the APSIM-Sugar model (Chapter 4).

5.1. Investigating the Capability of the APSIM-Sugar Model to Simulate Yield Differences Between Sugarcane Varieties Under Different Climatic Conditions (Chapter 2)

In Chapter 2 the capability of APSIM-Sugar to simulate the differences between biomass yields of four sugarcane varieties was investigated. The four varieties were grown under well irrigated and water stressed conditions as part of a breeding trial conducted at Home Hill, Queensland, Australia. Of the 89 varieties grown in the trial, the four varieties simulated were Q117, Q124, Q138 and R570 which are no longer grown for commercial production in Australia. The lack of a wider range of varieties in APSIM-Sugar highlighted the need for variety definitions in APSIM-Sugar to be updated. Simulated yields under well irrigated and stressed conditions were compared to observed yields. The effect of modifying the transpiration efficiency (TE) parameter (*transp_eff_cf*) was also investigated.

APSIM was unable to simulate the observed differences between variety yields and how these differences change when crops are grown under water stressed conditions. The difficulty in simulating yield differences highlighted the need for improved and updated variety definitions in APSIM-Sugar.

The parameter *transp_eff_cf* in APSIM-Sugar was a focus in this chapter because of the recent research of Jackson et al. (2014) that identified differences in transpiration efficiency between varieties and environments. Modifying *transp_eff_cf* had a large effect on simulated yields under stressed conditions. This suggests that APSIM-Sugar simulations could be improved by incorporating the latest physiological knowledge on genetic variation in TE. Chapter 2 was a significant contribution to the literature as no publications could be found beforehand that directly compared simulated differences between sugarcane varieties under different climatic conditions.

5.2. Investigating the Influence of Variety Parameters on Key Model Outputs Using Statistical Sensitivity Analysis (Chapter 3)

The focus of Chapter 3 was a global sensitivity analysis of APSIM-Sugar model outputs to variety parameters which extended on the investigation of TE reported in Chapter 2. A Gaussian Process was used to emulate the APSIM-Sugar model as an efficient method for global sensitivity analysis. The sensitivity of simulated biomass and sucrose yields to 14 parameters was analysed under well irrigated and water stressed conditions.

The results for the *transp_eff_cf* parameter accurately reproduced the results of Chapter 2 supporting the use of the GEM-SA software package used in the analysis. Parameters *min_sstem_sucrose_redn*, *tt_begcane_to_flowering*, *tt_flowering_to_crop_end* and *tillerf_leaf_size* were considered not influential ($S_i < 1$) while parameters *rue* and *transp_eff_cf* were the most influential parameters under well irrigated and water stressed conditions respectively. While rue and *transp_eff_cf* are difficult and expensive to measure directly, *leaf_size* and *green_leaf_no* are relatively cost efficient to measure and were influential under irrigated conditions. Collecting data on these two traits during breeding programs would help inform crop models such as APSIM-Sugar. Chapter 3 significantly contributes to the literature as no published sensitivity analysis for the APSIM-Sugar model or for sugarcane simulation models in general was available prior to this thesis.

5.3. Evaluating the Use of Two Bayesian Approaches to Statistically Calibrate Variety Parameters in the APSIM-Sugar Model (Chapter 4)

While parameters such as *leaf_size* and *green_leaf_no* were both influential and relatively simple to measure, the most influential parameters *rue* and *transp_eff_cf* are difficult and costly to directly determine in field experiments (Chapter 3). Chapter 4 presented an evaluation of two Bayesian calibration techniques that could be used to estimate values for such parameters. Ten parameters identified as influential in Chapter 3 ($S_i > 1$) were calibrated in Chapter 4.

Generalized Likelihood Uncertainty Estimation (GLUE) and Markov Chain Monte Carlo (MCMC) were used to calibrate APSIM-Sugar in a theoretical and real world evaluation. In the theoretical evaluation GLUE and MCMC calibrated APSIM-Sugar for two pre-defined varieties. This evaluated the ability of the calibration methods to approach known parameter values for different varieties. The real world evaluation was based on GLUE and MCMC calibration of variety Q117 using observed yields allowing for a realistic evaluation of calibration uncertainty and validation against observed data not used in calibration.

Both GLUE and MCMC were able to accurately estimate the known variety parameters in the theoretical evaluation with parameter estimates differing accurately between the two pre-defined varieties (V001 and V002). This included parameters that are difficult to measure directly such as *transp_eff_cf*, *rue* and k_L. The theoretical analysis identified parameters that were difficult to estimate accurately such as *sucrose_delay*. Using the analysis from Chapter 3 it was possible to hypothesize why certain parameters were difficult to estimate. This highlights the importance of understanding how parameters to be calibrated will actually influence model outputs. The theoretical analysis provided valuable insights in the use of statistical calibration techniques and support their use in calibrating variety parameters in the APSIM-Sugar model.

When applied to the well documented variety Q117, parameter values estimated by GLUE and MCMC differed. Differences were also found between estimated values and default values for certain variety parameters. Despite this, simulated green biomass and sucrose yields using either GLUE or MCMC calibrations were as or more accurate than an application of the default parameter values. Although there was little difference in the performance of GLUE and MCMC calibrations, MCMC produced slightly better results in the real world validation and had a range of supporting statistics to assess the convergence and stability of the estimated posterior distribution. Prior to this study there was no available published analysis that had used Bayesian statistics to calibrate the APSIM-Sugar model for variety parameters. The analysis presented in Chapter 4 makes advances on earlier research that has applied GLUE to a sugarcane crop model by identifying strengths and weaknesses in different Bayesian statistical approaches before they are used to calibrate new varieties.

5.4. Future Work and Final Remarks

Variety parameters in APSIM-Sugar can now be routinely updated as new varieties are released. It is recommended that modellers use the methodological framework developed in this thesis to do so regularly. Results presented in Chapter 4 suggest that Bayesian statistical parameter estimation techniques can be used to estimate values for parameters that are difficult to measure using a limited amount of data which are routinely collected in breeding programs. Future research could consider more advanced adaptive MCMC algorithms to improve calibration efficiency. Calibration performance could also be improved by removing parameters with a relatively weak influence on model outputs such as *sucrose_delay* and k_L and using observed values for parameters such as *leaf_size* and *green_leaf_no* which are relatively easy to measure in the field compared to parameters such as *transp_eff_cf* and *rue*.

Identifying parameters for future calibrations could be improved by extending the research reported in Chapter 3. Future global sensitivity analysis can be performed for a wider range of environments to which the crop will be exposed. As parameter values can differ between crop classes (plant or ratoon) future work could also consider the effect of crop class on parameter sensitivity. As APSIM-Sugar can now be calibrated for new varieties, it will be necessary to show that simulated differences between varieties accurately represent observed differences for a range of growing environments. This will build confidence in the use of new variety definitions for investigating variety, environment and management interactions.

The ability to investigate variety, environment and management interactions will help improve APSIM-Sugar in its role as a decision support tool. On a regional level this could include improved regional yield forecasts. At a farm level management programs could be designed for specific varieties grown in specific paddocks. Furthermore, the tools developed for this thesis in the R statistical program (available on request) provide researchers with a method for manipulating APSIM-Sugar varietal parameters making trait simulation studies such as sensitivity analysis more accessible. The Bayesian techniques applied in this thesis have not previously been available for APSIM-Sugar but have proven to be useful tools and will play an important role in further developing the simulation capabilities of the sugar industry.

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