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INVITED

A method to improve the efficiency of calibrating biophysical models for pastures

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Abstract: Parameterisation of biophysical models to represent pasture species is a time consuming and complex process. Various pasture plant species of commercial interest have been developed and are available as calibrated plant models in the GRAZPLAN ruminant grazing systems model, but capacity to improve existing or develop new species is limited. Our study reports the implementation of an optimization method to parameterise pasture in AusFarm, a product of Grazplan, with a case study of kikuyu, a sub-tropical perennial grass. The Parameter ESTimation (PEST) calibration method was used to generate new plant species parameters for kikuyu, and the accuracy of predictions based on original and new parameters were compared. While the error values for line of best fit were similar for observed versus simulated values for both original and new plant parameters, the accuracy of predictions was improved correcting a substantial under-estimate in the simulated values using the original plant parameters. The results of PEST optimisation of a pasture plant might also be used to identify the presence and source of biological constraints in pasture trials, although this hypothesis was not tested. Our preliminary application of the PEST optimisation process to improve pasture plant biophysical models, demonstrates the potential for improved efficiency in the development and calibration of new pasture plants, particularly for cases where a relevant base model for the species exists.

Keywords: *Pasture, plant model, GRAZPLAN, kikuyu, PEST, Parameter ESTimation*

1. INTRODUCTION

GRAZPLAN biophysical modelling is widely used to represent pasture and livestock production systems in southern Australia (Moore et al. 1997). This modelling framework includes plant species that represent most of the common pasture types grown in this region, both annual and perennial. Relatively more recently C4 grass models have been developed and used to model scenarios that add to field research activities carried out in Western Australia and South Australia (Sanford 2013; Descheemaeker et al. 2014).

Effective parameterisation of models of pasture plants ensures that the models accurately simulate the growth and development of the target plant species under different environmental conditions and management regimes. The calibration of plant species models is an intensive process, and they are often generated for a limited range of experimental conditions. Each pasture species is parameterised by up to 250 individual parameters which aim to individualise its behaviour and decouple it from geographical biases and ensure that it behaves in a generic fashion driven only by the climate and soil inputs to the pasture model.

To apply biophysical pasture models more broadly, it is important to ensure model parameters are calibrated to reduce parameter uncertainty, and thereby the uncertainty of simulation results. This paper reports the implementation a method for re-calibrating existing plant species as data becomes available for new locations and field conditions.

2. METHODS

The Parameter ESTimation (PEST) calibration method (Doherty et al. 2011) was applied as a case study for the GRAZPLAN kikuyu model, using pasture plot trials that were conducted in New South Wales (Kemp 1975; Neal et al. 2009). Kikuyu is a perennial C4 sub-tropical grass, that is commonly used as pasture for livestock around the world (e.g. Swanepoel et al. 2015). In summary, the plot trials were for kikuyu grass established by seed in spring and allowed to establish in the first year. In the second year following their winter dormancy, swards were cut at intervals and their production of biomass was recorded. The trials were i) rainfed with 68 kg/ha N applied after each of the 10 cuts per year (Kemp 1975) and ii) irrigated with rates of N, P, K, Mg, S applied to ensure nutrients did not limit growth, confirmed by leaf tissue testing (Neal et al. 2009).

The workflow had four main components:

1) Developed a Microsoft® Excel-based GUI for automating the set-up of PEST calibration process.
2) Identified plant model species parameters that were sensitive to plant growth simulation.
3) Applied PEST automatically set up via the GUI to calibrate the model species parameters identified in step 2.
4) Compared predictive skill of existing and optimised kikuyu models.

The PEST program is a model-independent parameter estimator with model calibration and advanced predictive analysis features. In this study, PEST was integrated with the AusFarm model (Moore et al. 2007) to derive the values of the pasture species parameters for simulating pasture biomass. For a given set of parameters, PEST will adjust model parameters until the fit between the model outputs and measurements are optimized by minimising the sum of squared deviations between model-generated values and experimental observations. The Gauss-Marquardt-Levenberg algorithm (GML) method is used in PEST to optimize the model parameters, which has the most notable pronounced advantage to complete a parameter estimation process with an extremely high level of model run efficiency. The PEST optimisation interacts with simulation models such as AusFarm to re-run scenarios as many times as required to adjust the parameters for minimising the discrepancies between simulated and observed values for harvested biomass in this study. Further details on PEST can be found on the website of http://pesthomepage.org/ and (Doherty et al. 2011).

For optimizing parameters, users need to select parameters, prepare initial and boundary values for the selected parameters and read observed data to set up PEST files. To facilitate this process, an Excel-based tool was developed to automate the process of setting up the PEST file (Figure 1). Using the Excel-based tool, the AusFarm parameter file is read by clicking the tab of "Read prm file"; the parameters that the users would like to optimize can be selected by clicking the tab of "Select parameters"' the observed data can be read into PEST file by clicking the "Read observation data; the instruction, template and pest files that PEST requires can be created using the functions of "Create ins file ", "Create tpl file" and "Create pst file", respectively.

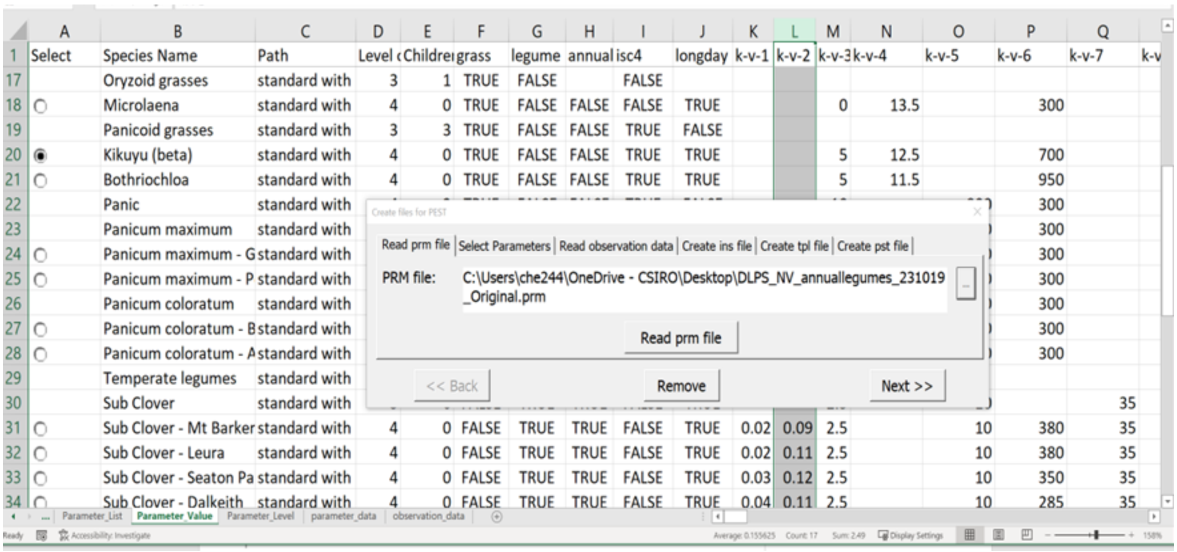


Figure 1. The interface of an Excel-based tool to automate the setting up the PEST file

For the case examined in this study, a sensitivity analysis showed that 8 parameters in AusFarm are sensitive to the simulations of the growth of kikuyu (Table 1). The initial parameter values for optimization were set up as the current values in AusFarm, with the minimum and maximum values set based on the range of feasible values for each parameter.

Table 1. Existing and newly optimized values for selected sensitive parameters in the kikuyu plant model

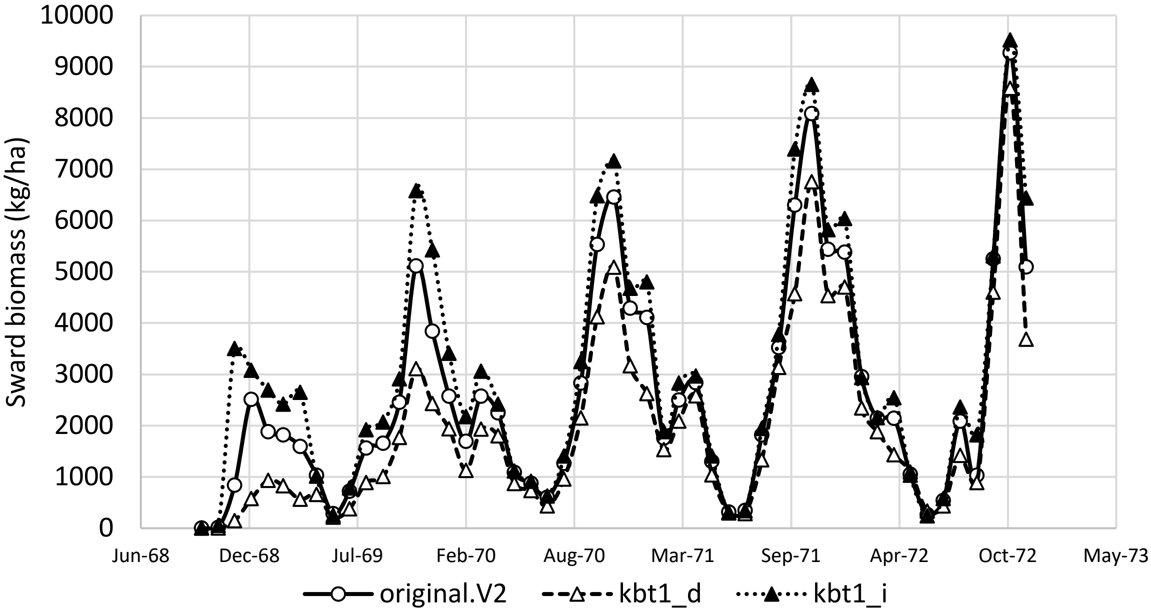
Parameter	Description	Original values	New values	% change
k-i-1	Reference specific leaf area (ratio of leaf area index to leaf weight)	0.03	0.021	-43
k-i-2	Reference specific stem area	0.005	0.006	17
k-i-7	Apparent light extinction coefficient under ungrazed conditions	0.55	0.444	-24
k-i-8	Apparent light extinction coefficient under heavily defoliated conditions	0.8	0.284	-182
k-ru-1	Radiation use efficiency under reference conditions	4.0	4.078	2
k-ru-3	Relative photosynthetic efficiency of stems	0.3	0.965	69
k-bt-1	Biomass transpiration coefficient	12.0	11.908	-1
k-hr	Height ration: also governs the size of the ungrazeable portion of the plant	1.0	0.949	-5

3. RESULTS

Sensitivity analyses were conducted across candidate parameters from the GRAZPLAN pasture model, using AusFarm. Graphs used to evaluate parameter sensitivity are shown in Figure 2, using plot trial data from Kemp (1975) that was aggregated monthly. In these examples, harvested biomass was strongly sensitive to the biomass transpiration coefficient (k-bt-1) but very weakly sensitive to the maximum rate of front root extension (k-r-2), which was subsequently excluded from the PEST optimisation. Sensitive plant model parameters for use in PEST optimisation were identified by visual assessment, evaluating whether changing the parameter in isolation produced a substantive change in prediction of harvested biomass.

The optimisation of plant model parameters markedly improved the accuracy of simulation modelling predictions for the Neal et al. (2009) data. Figure 3 shows a large under-prediction of harvested biomass, aggregated at 3-monthly intervals, based on the original parameters. However, seasonal patterns of harvested

(a)



(b)

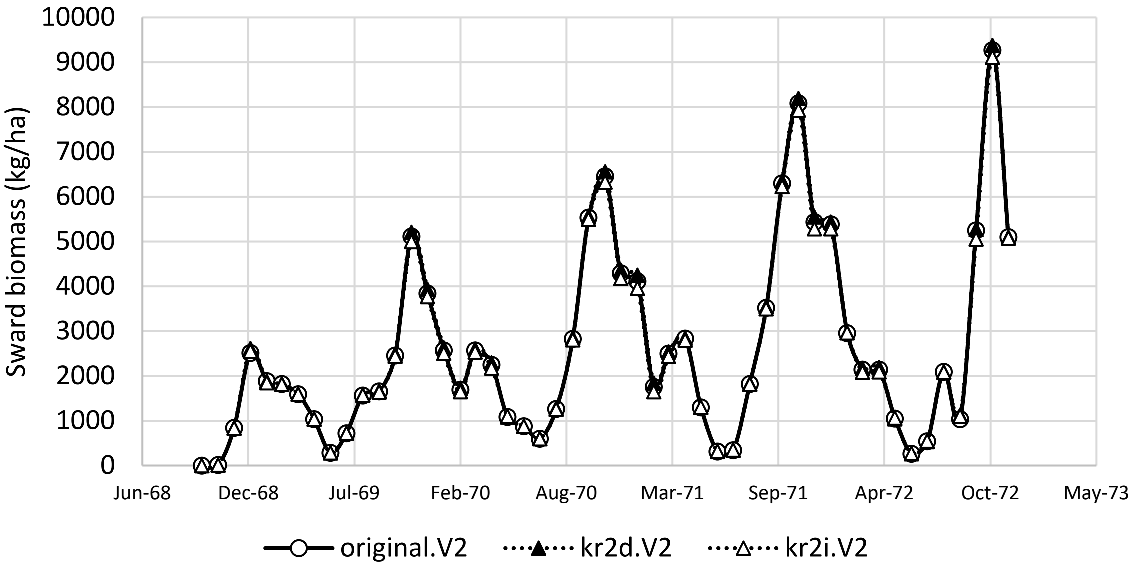


Figure 2. Example of parameter sensitivity analyses using original (○) or test (▲) values for (a) kbt1 and (b) kr2 parameters for prediction of sward biomass

biomass corresponded closely with the observed data using the optimised plant model parameters (Figure 3). The improvement in model prediction is further illustrated in Figure 4, with the slope of the line of observed versus simulated values of 0.26 (R^2=0.829) for original parameters, compared with 0.92 (R^2=0.896) for the new plant model parameters.

New calibrated values for the 8 kikuyu plant model parameters selected for PEST optimisation based on Neal et al. (2009) data, and percentage change from original values, are shown in Table 1. This process identified apparent light extinction coefficient under heavily defoliated conditions (k-i-8) and the relative photosynthetic efficiency or stems (k-ru-3) as the most sensitive plant model parameters of those tested. Other parameters such as radiation use efficiency (k-ru-1), biomass transpiration coefficient (k-bt-1), and height ratio (h-hr) values remained similar to the original parameters.

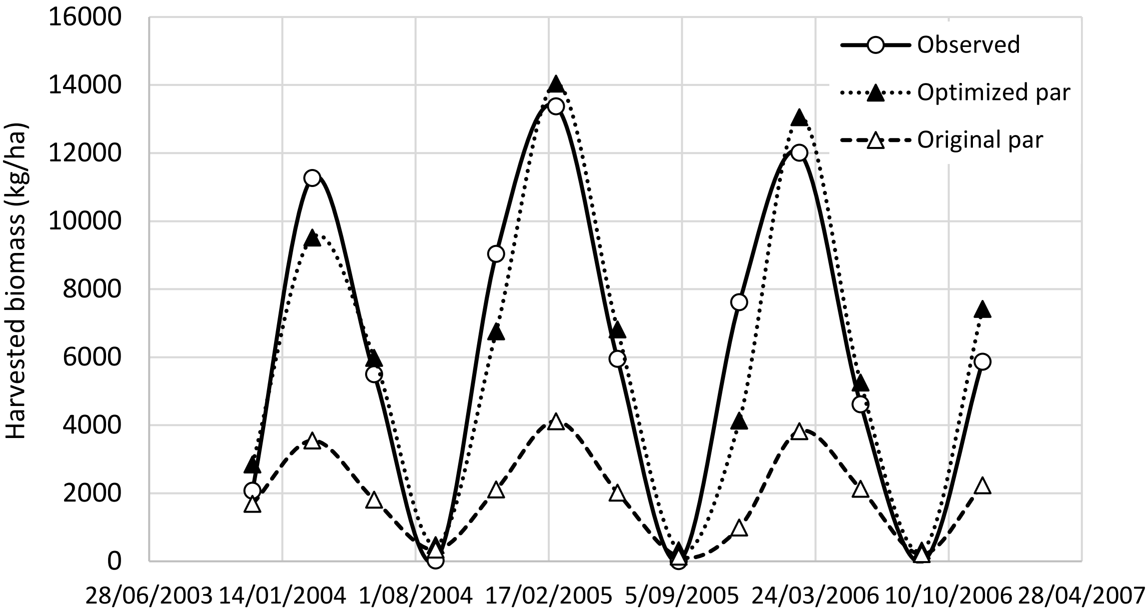


Figure 3. Comparison of observed and original (○) or optimized (▲) estimated values of pasture biomass (aggregated over 3 months) for the kikuyu plant model

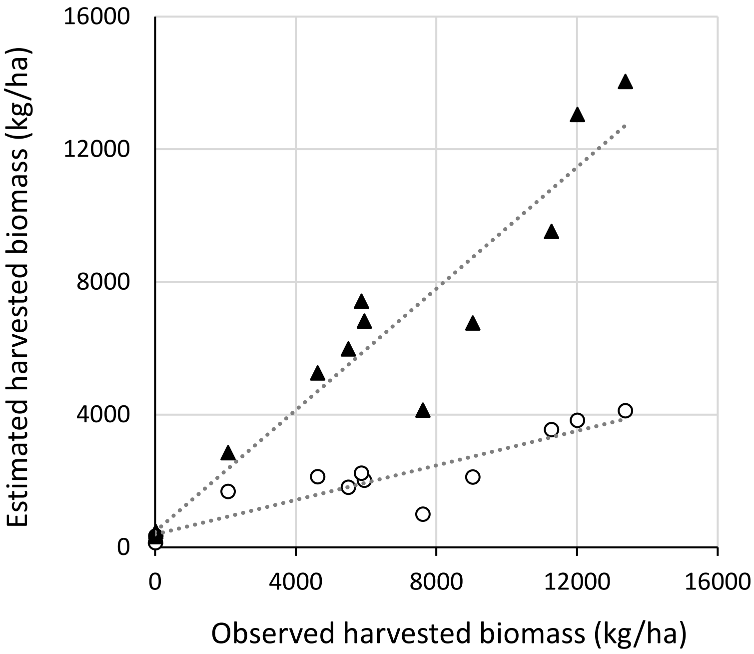


Figure 4. Comparison of observed and simulated biomass (aggregated over 3 months) of kikuyu pasture with original (○) or optimized (▲) plant species parameters

4. CONCLUSIONS AND RECOMMENDATIONS

In this paper we demonstrated an efficient method for calibration of biophysical plant model species, by applying the PEST optimisation tool in AusFarm with the kikuyu sub-tropical grass model. We showed that the accuracy of prediction can be improved substantially for a pasture modelling scenario. While this does not necessarily mean that in this case the model will be improved more broadly, these results suggest this would be the case with the availability of adequate training data. Given that there were biological constraints identified in the field study where the existing model performed well, it is possible that the new parameters would better represent kikuyu more generally, but this remains to be tested.

Identifying the sensitive plant model parameters to include in optimisation is a critical first step in the implementation of the PEST method. In this case we have used a reasonably simple experimental model for use in calibration, i.e. harvested plot trials. More complex management scenarios, e.g. grazing or carbon balance, will likely necessitate use of a larger parameter set for calibration of plant models to account for additional factors such as plant-animal interactions such as selective grazing of plant components or plant-soil interactions such as soil carbon fluxes (Thomas et al. 2012). However, the parameters that were identified as sensitive in this study would likely be the same for other pasture plot trial scenarios for sub-tropical grasses.

The PEST optimisation process quantified the extent to which the selected parameters were adjusted in the optimisation process. This may have some biological relevance, highlighting experimental factors and biological constraints that may have been present in the field data. For example, predicted harvest biomass based on original parameters was reasonably accurate for the Kemp (1975) data, but produced a substantial under prediction of harvest biomass for the Neal et al. (2009) plot trials. This identifies the possibility of biological constraints to kikuyu growth in the Kemp (1975) study, which was suggested by the author.

Improvements in the accuracy of biophysical pasture models has become increasingly important, as they are used to generate information for digital agriculture products (Herrmann et al. 2021; Mitchell et al. 2022). The ongoing integration of domain expertise with advanced analytics and data tools is essential to ensure these emerging digital products are well supported and deliver the highest value to the agricultural industry.

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