Bayesian Calibration of AquaCrop Model

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Abstract: The AquaCrop simulation model, modelling the dynamic change of crop growth status, is an important crop management tool for quantifying crop yield response to water. To effectively simulate the soil water balance and the crop growth process, a number of system parameters and canopy state variables are inevitably adopted. As a result, certain key parameters need to be calibrated so that the AquaCrop model can achieve a better performance of prediction for various scales of regions. This paper aims to apply Bayesian technique to calibrate the AquaCrop model. In this approach, the prior information regarding the system parameters is expressed in the form of a uniform probability distribution. Then with the advent of output variable measurement (e.g. biomass) by remote sensing techniques, the parameter distributions are iteratively updated by using Bayesian Markov Chain Monte Carlo (MCMC) method. The calibrated system parameters are expressed by the posterior distributions and gained by distribution mean value. Finally, the Bayesian calibration is compared with the conventional optimisation based calibration in terms of biomass and canopy cover, where simulated annealing is chosen as the optimisation approach, indicating a better calibration performance can be achieved by using Bayesian methods. Consequently, it is recommended that Bayesian calibration is one promising approach to the problem of crop model calibration.

Key Words: Bayesian method, AquaCrop model, parameterisation, data assimilation

1 Introduction

Precision agriculture is increasingly developed to improve the work efficiency and crop productivity due to the rapid development of modern techniques, such as remote sensing, machine learning and crop simulation model [1-2]. It is necessary to pay more attention to national food security and sustainable agricultural development with increased concern for the improvement of agricultural predictive parameters because the increasing population require huge food consumption, and on the other hand, to reduce the waste of water during planting process. Crop models are tools for explaining and predicting crop physiological growth by adopting mathematical formulations under different stresses [2].

Due to the characteristics that crop growth models are usually based on the crop photosynthesis, transpiration, respiration, nutrition, there is a demand for an approach, applicable to crop models that quantifies output uncertainties, identifies sensitive parameters and variables to improve model prediction performance in various scale fields [3-4]. Therefore, in most cases, crop growth model integrated with remotely sensed data from diverse remote sensing platforms has been an effective method to calibrate model input parameters and predict processed variables (state variables change with time e.g. biomass or canopy cover) and final variables (e.g. yield).

The Agricultural Model Intercomparison and Improvement Project (AgMIP) indicated that poor prediction performances may be obtained when one crop model applied in different fields, due to uncertainties in the spatial distribution of soil parameters, crop parameters and field management [4-5]. These uncertainties of crop growth model can be reduced by using more information to improve model parametrisation and calibration, and increase the final data assimilation accuracy.

Data assimilation has been known as a mainstream approach for crop growth and yield prediction by integrating crop model and remote sensing data. optimisation based calibration is one of the data assimilation methods where some uncertain model parameters are optimised by minimising the processed variables differences between the model based prediction and the observed data in recent years [6-7]. For example, Jin adopted particle swarm optimisation algorithm to calibrate input parameters to improve the yield prediction accuracy combining AquaCrop model and multi-sources remote sensing data [8-9]. Xing compared three optimisation methods for AquaCrop model calibration and concluded that shuffled complex evolution (SCE) algorithm is better than particle swarm and simulated annealing algorithm on this model for agricultural applications [10].

In comparison with optimisation based model calibration, Bayesian model calibration method has been widely applied in a number of areas due to its fine properties, such as posterior distribution estimation and global solution. The main purpose of Bayesian approach is to quantify the inputs and outputs of models by probability distributions and adopts the rules of probability theory to update the distributions when observed data are available [11-12]. It is deeply related to the analysis of prior data to select the probabilistic models. Whyte calibrated cancer natural history model by adopting Metropolis-Hastings algorithm from posterior distribution and obtained a good fit to all observed data [11]. Oijen calibrated forest models and concluded that Bayesian calibration methods can be applied to all types of process-based forest models with a high efficiency [3]. Hinsbergen adopted Bayesian theory to calibrate car-following model and proved it is one promising tool for quantitatively analysing inter-driver differences [12].

The new water driven crop model, AquaCrop, with characters of simplicity, robustness, accurateness, was proposed in 2009 by Steduto showing better results in predicting crop growth status, especially in irrigated regions [13]. According to the principle of AquaCrop model, Foster developed it into an open-access called AquaCrop-OS which can avoid a compiled software problem and be linked with other disciplinary models quickly to support yield estimation, water re-

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source management and intelligent irrigation program from 2016 [14]. AquaCrop-OS is one Matlab programmed software and has been proved to be able to get a corresponding performance with AquaCrop model experimenting on wheat, cereals and potatoes by Foster [15].

Previous researches have been mainly focused on adopting optimisation based method to calibrate crop model integrating crop model and remotely sensed information so that a better prediction can be guaranteed (see [6-9]). However, little has been done to calibrate AquaCrop model by using Bayesian method. Consequently, AquaCrop-OS parameters will be calibrated by using biomass measurement data in this paper as a case study. And, state variable canopy cover will also be adopted to show the prediction performance. Our goal in this paper is to demonstrate how a Bayesian approach provides a logical method for calibrating AquaCrop model and compare the optimisation based calibration results with Bayesian calibration results. The remaining part of this paper is organised as follows. The superiority of Bayesian calibration compared with optimisation based calibration is described in Section 2. Calibration methodology is discussed in Section 3, including data sources and calibration process. Bayesian calibration results are presented and compared with optimisation calibration results in Section 4. Finally, conclusions are drawn in Section 5 with future work.

2 Bayesian calibration

Calibration is the process of inferring the model parameters from the data on the model outputs. However, output variables may not be accurate and comprehensive to allow exact inference of parameters values [3]. The optimisation approach for crop model calibration aims to find a combination of parameters that minimises an objective function J. Various types of objective functions have been considered in the literature, although most often it is defined by the sum of the squared differences (SSE) or root-mean-square error (RMSE) between model based prediction data and observed data (remote sensing acquisitions). It is assumed that the output state variables generated by parameters producing the minimal error is the optimal estimate of the parameters. Normally, optimisation methods employ an iterative process, where the objective function is minimized by adopting various update rules, to find an optimal point [16]. In crop model calibration area, several optimisation calibration methods have been used in this research for a long time, including simplex search algorithm, Least Squares Method (LSM), Shuffled Complex Evolution (SCE), Very Fast Simulated Annealing (VFSA) and Particle Swarm Optimisation Algorithm (PSO) [17-20]. These kinds of methods only provide a single point of estimate of parameters and may get stuck in an incorrect local minima [16].

Bayesian approach for crop model calibration allows probabilistic consideration accounting for uncertainties in input data. In this approach, prior information on system parameters can be easily accommodated, yielding a better parameter estimate. Besides, the Bayesian approach is in seeking not only for finding an optimal point but obtaining the probability density function of the estimated parameters. For this reason, Bayesian calibration is one calibration process updating probability distributions of uncertain parameters with the advent of output variable, which differs from optimisation based parameters "tuning"(i.e. obtaining the best parameter combinations maximising the fit between model outputs and observed data).

3 Methodology

Our approach is to integrate the crop model AquaCrop-OS and simulated observations (Gaussian noise added to the model output groundtruth variable) to estimate most sensitive parameters and output state variables (biomass) through Bayesian theory based on Markov Chain Monte Carlo (MCMC) techniques. After setting the prior probability distributions of sensitive parameters and the likelihood functions for the output variable, the posterior distributions of calibrated parameters can be generated by running AquaCrop-OS model repeatedly referenced by MCMC scheme [11].

3.1 Bayesian calibration framework

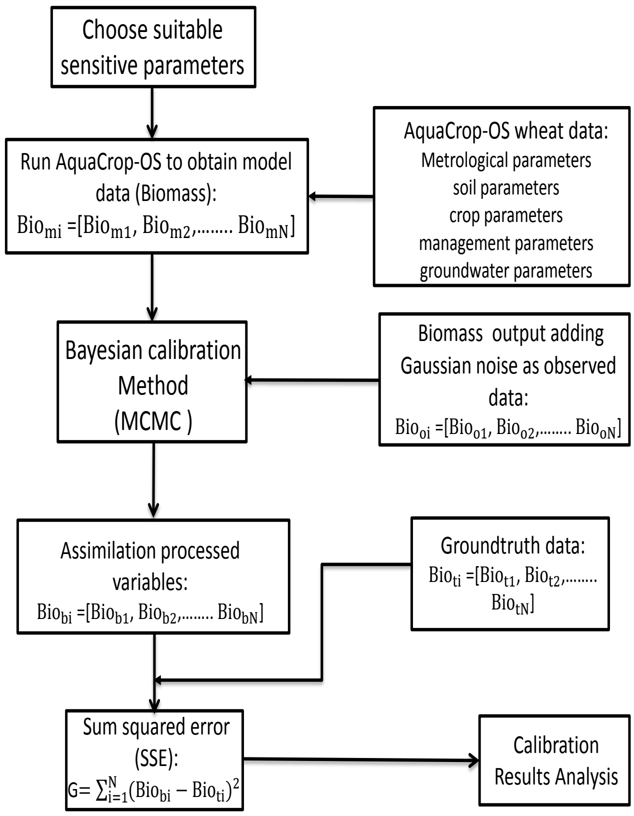

Fig. 1: Bayesian calibration framework

The Bayesian calibration framework is shown in Fig. 1. The whole process consists of model data acquisitions, observed data acquisitions, data assimilation (Bayesian calibration method) and results analysis part. Data acquisitions are in preparation for data assimilation process, and results analysis will present the Bayesian calibration results with groundtruth. The AquaCrop-OS model run by default crop parameters is described as the groundtruth. Model data are generated by AquaCrop-OS using various crop parameters and Gaussian noise is added to the output state variable groundtruth data (biomass) as observed data. Sum squared error (SSE) is set as an indicator to analysis calibration results by using calibrated biomass and groundtruth biomass, given by:

$$G = \sum_{i=1}^{N} (Bio_{bi} - Bio_{ti})^2 \quad (1)$$

where Bio_{mi} denotes the model biomass generated by wide range of parameters, Bio_{oi} means observed biomass from remote sensing platforms. Bio_{bi} is the Bayesian calibrated biomass and Bio_{ti} represents groundtruth biomass.

3.2 AquaCrop model

Steuto proposed the water driven crop model with well-properties (simplicity, robustness, accurateness) in 2009. The relationship between crop yield and crop transpiration under diverse stress can be simulated by AquaCrop model [13]. The crop's daily aboveground biomass was generated by normalised crop water productivity ($NCWP$) from the AquaCrop model [8]. Biomass yield was determined by $NCWP$ and the ratio of crop transpiration (ET) and reference evapotranspiration (ET_0) via Eq. 2, and grain yield (Y) was obtained by multiplying the harvest index (HI) by the biomass yield (B) (see Eq. 3).

$$B = NCWP \times \sum \frac{ET}{ET_0} \quad (2)$$

$$Y = B \times HI \quad (3)$$

where $NCWP$ is the normalised crop water productivity in g/m^2; ET is crop transpiration in mm; ET_0 is the reference evapotranspiration in mm; B is biomass yield in ton/ha; HI is the harvest index; and Y is grain yield (ton/ha).

Foster developed it into AquaCrop-OS on the basis of AquaCrop model [14, 15]. AquaCrop-OS has the same file as AquaCrop, but is programmed by Matlab software. Input and output files are stored as text files in AquaCrop-OS folder. Input folder consists of five main parts to be set: metrological parameters, soil parameters, crop parameters, management parameters, and groundwater. Output folder includes four parts: water contents, water fluxes, crop growth and final output files. Input files are parameters and output files are processed variables and final variables when time changes, which means output state variables can be inserted into data assimilation program. The uncertain parameters to be calibrated in this paper are stored in crop parameters file.

3.3 Markov chain Monte Carlo (MCMC)

Bayesian calibration aims to derive the posterior probability distributions for parameters of interest conditional on output variables, where the parameter posterior distribution $p(\theta|D)$ is proportional to the prior parameter distribution $p(\theta)$ and the measurement likelihood function $p(D|\theta)$, given by:

$$p(\theta|D) \propto p(\theta) \times p(D|\theta) \quad (4)$$

where θ denotes the parameter vector to be calibrated and D represents the observed data. The likelihood function $p(D|\theta)$ evaluates each value for θ based on how well the model with parameter θ is able to reproduce the data D. In this work, the differences between the observed data and model data are attributable to measure error in D and the likelihood function is assumed to be a Gaussian distribution with a proper covariance matrix with the following form:

$$p(D|\theta) = p(E = D - M(\theta)) \quad (5)$$

where $M(\theta)$ represents the computed model output data given a candidate value for parameter θ, and E denotes the error between measurement outputs and process model outputs with parameter θ (i.e. measurement error for $M(\theta)$).

To effectively estimate the posterior distribution, a Markov Chain Monte Carlo (MCMC) algorithm entitled Metropolis-Hastings algorithm is adopted. Metropolis-Hastings algorithm is to obtain a sequence of random samples for a probability distribution for which direct sampling is difficult. In this approach, a sequence of samples is iteratively generated to approximate the desired distribution. At each iteration, the algorithm selects a candidate for the next sample value based on the current sample value (forming a Markov chain), where the candidate is either accepted or rejected with some probability.

Remark: The prior information $p(\theta)$ reflects our prior knowledge on the parameters, which may come from past experience or expert knowledge. If poor prior knowledge is available, a distribution with a large covariance matrix can be chosen and the posterior distribution will be dominated by the data and vice versa [11-12, 16-18].

3.4 Data Sources

From reference [21, 22], crop and soil parameters in AquaCrop model was researched by using a sensitive analysis adopting Extended Fourier Amplitude Sensitivity Test (EFAST) under different environment and conditions for various crops and soil to determine the sensitive parameters during the period of growth. Jin applied eight sensitive parameters in his study to predict yield production [8, 9]. From literature, the normal procedure for calibration is to fix insensitive parameters and adjust the sensitive parameters when the model is localised. The range of six parameters to be calibrated in this paper with high sensitivity is shown in Table 1.

Table 1: Range and groundtruth of sensitive crop parameters to be calibrated

Parameter	Range	Groundtruth
Canopy growth coefficient (cgc)	0.05–0.07	0.065
Maximum canopy cover in fraction soil cover (ccx)	0.82–0.99	0.94
Canopy decline coefficient (cdc)	0.04–0.07	0.05
Growth degree day from sowing to emergence (eme)	50–200	80
Shape factor for water stress coefficient for stomatal control (pstoshp)	1.5–3.5	2.5
Growth degree day from sowing to maximum rooting depth (rootdep)	1300–1600	1400

Groundtruth acquisition: Groundtruth is of high importance during the process of crop model calibration. AquaCrop-OS model has its default crop and soil parameters stored in input files. Biomass is set as the state variable output (see Fig. 2). In our case, the default crop parameters of AquaCrop-OS with high sensitivity are treated as groundtruth parameters inputs (see Table 1).

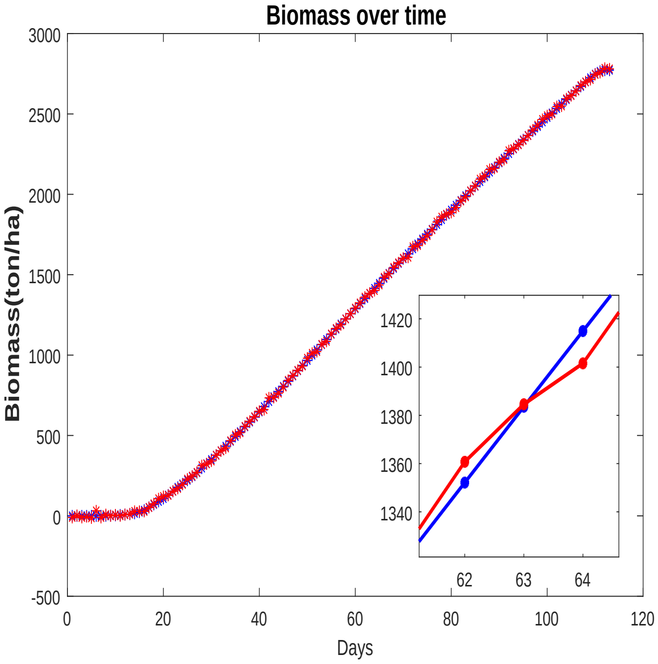

Fig. 2: Groundtruth and observation of biomass data over time

Observed data and model data acquisitions: Gaussian noise added to AquaCrop-OS model state variable output biomass is to simulate an observed data from remote sensing platforms. After adding the noise (mean=0; variance=100) to the biomass in output file, an observed biomass with respect to time can be obtained (see Fig. 2). Biomass of model data are generated under various sensitive crop parameters with the range and compared with observed data using Bayesian method to obtain calibrated parameters posterior distributions.

3.5 Bayesian calibration process

Sensitive parameters to be calibrated have been listed in Table 1. The AquaCrop-OS model can quickly be run to produce output of biomass data for a given range of parameters. Our Bayesian based calibration used the Metroplis-Hasting (MH) to generate multiple sets of parameters from the posterior distribution.

In our case, our simulated days are set as 112, θ is defined as: θ = [cgc, ccx, cdc, eme, pstoshp, rootdep] and D includes the simulated observed data from remote sensing platforms (see section 3.4). The flowchart of steps by Metropolis-Hasting algorithm is shown in Fig. 3. At the beginning of the crop model calibration, the independent uniform distributions with the upper and lower bounds of sensitive parameters are adopted as prior information and the initial parameters are randomly chosen. From the current set of parameters, a set of proposal parameters is obtained by taking a step randomly in the parameter space. The likelihood of both the current set and the proposal set compared with the given observation data is to determine whether the proposal set will be accepted or not [11]. The decision to accept or reject the proposal parameter set is based on the consideration of the ratio of the posterior probability distribution at the proposed location, to the previous location. The current parameter set will be replaced by the proposal parameter set as a new current set once the proposal parameter set is accepted, otherwise, the current parameter set will be repeated in the chain again. The aims of the whole process using MH algorithm is to get a chain of parameters set after maximum repeat times [11].

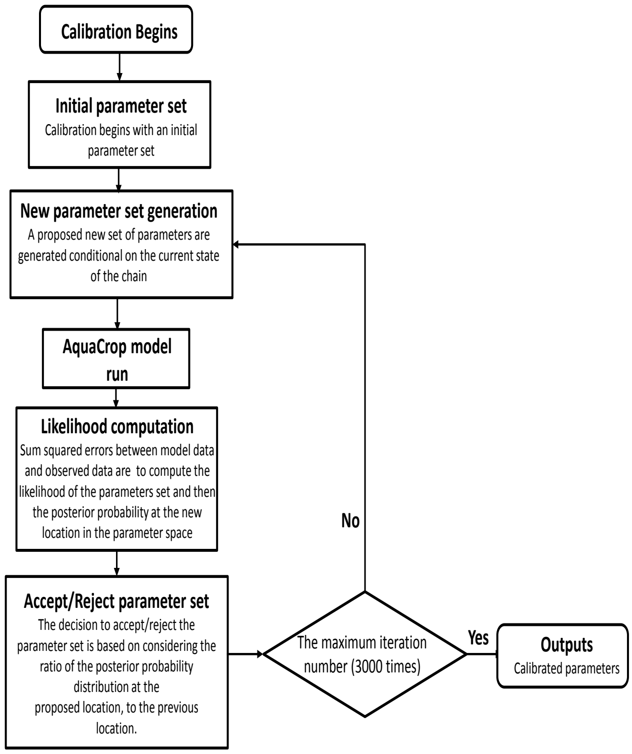

Fig. 3: Flowchart of steps by Metropolis-Hasting algorithm

Table 2: Bayesian and optimisation calibrated parameters with the observation of biomass

Parameter	Optimal result	Bayesian result
Canopy growth coefficient (cgc)	0.0500	0.0506
Maximum canopy cover in fraction soil cover (ccx)	0.9026	0.9284
Canopy decline coefficient (cdc)	0.0509	0.0481
Growth degree day from sowing to emergence (eme)	67	66
Shape factor for water stress coefficient for stomatal control (pstoshp)	1.6496	2.1113
Growth degree day from sowing to maximum rooting depth (rootdep)	1358	1422

4 Results

Calibrated sensitive parameters are in the form of posterior distribution after adopting Bayesian theory and the final parameters are obtained by distribution mean value. The simulated annealing optimisation calibration method is compared with Bayesian calibration method on parameters in Table 2.

For a real experiment, it is inconvenient to compare the calibrated parameters with the groundtruth parameters, thus, the evaluation of calibrated parameters will be conducted by state variable output: biomass. Groundtruth biomass and calibrated biomass is calculated by using sum squared error (SSE). Moreover, calibrated canopy cover by Bayesian method will also be compared with optimisation method. The error of the calibrated biomass and canopy cover by optimisation and Bayesian methods in comparison with the groundtruth can be described from Eq. (6) to Eq. (9).

$$E_{bo} = \sum_{i=1}^{N} (Bio_{opt} - Bio_{truth})^2 \tag{6}$$

$$E_{bb} = \sum_{i=1}^{N} (Bio_{Bay} - Bio_{truth})^2 \tag{7}$$

$$E_{co} = \sum_{i=1}^{N} (CC_{opt} - CC_{truth})^2 \tag{8}$$

$$E_{cb} = \sum_{i=1}^{N} (CC_{Bay} - CC_{truth})^2 \tag{9}$$

where Bio_{opt} and Bio_{Bay} indicates calibrated parameters applying to biomass by optimisation method and Bayesian method, respectively. CC_{opt} means state variable canopy cover generated by AquaCrop-OS model using optimisation calibrated parameters and CC_{Bay} means state variable canopy cover generated by AquaCrop-OS model adopting Bayesian calibrated parameters. Bio_{truth} and CC_{truth} represents the default groundtruth of biomass and canopy cover. N is the simulated days.

Table 3: Sum squared error of calibrated canopy cover and biomass by using optimisation based calibration and Bayesian based calibration

State variable	Optimisation error	Bayesian error
Canopy cover (CC)	0.2238	0.0658
Biomass (Bio)	4573.1	163.5

The error of Bayesian calibrated biomass and the groundtruth is 163.5 and the error of optimization based calibration is 4573.1, much larger than Bayesian calibration error (see Table 3). The error of Bayesian calibrated canopy cover and the groundtruth is 0.0658 and the error of optimization calibrated canopy cover and the groundtruth is 0.2238, which shows calibrated canopy cover also obtains a corresponding result as calibrated biomass.

Additionally, from Fig. 4 and Fig. 5, it is obvious that biomass or canopy cover employing Bayesian calibrated parameters (pink line) outperform optimisation based calibration results (green line) as Bayesian line is much closer to the groundtruth (blue line).

5 Conclusion

In this study, we conducted Bayesian calibration method applying to AquaCrop crop model and compared this

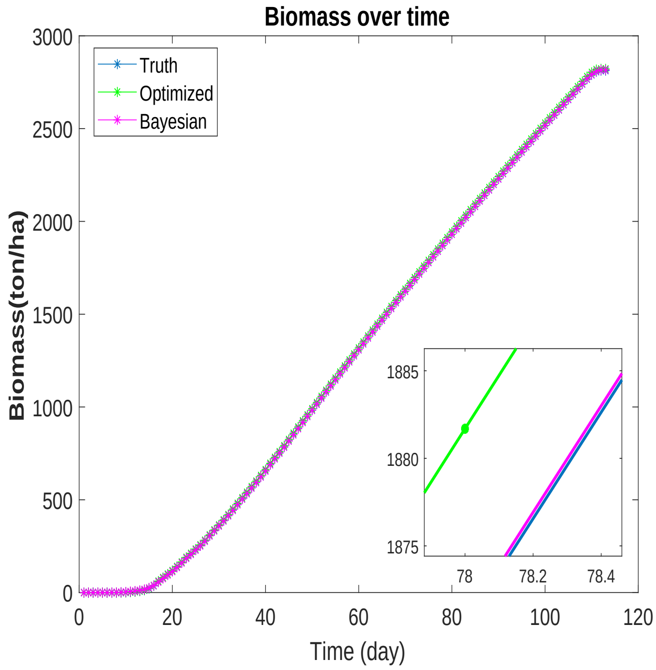

Fig. 4: Optimisation and Bayesian calibration results with the measurement of biomass

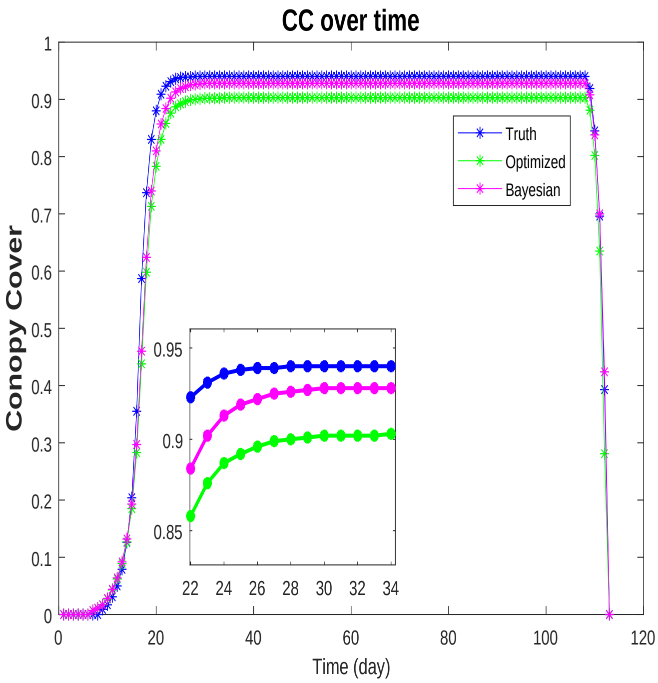

Fig. 5: Optimisation and Bayesian calibration results with the measurement of canopy cover

method with conventional optimisation based calibration where simulated annealing is chosen. As can be seen from this simulation, the parameter distributions are iteratively updated by using Bayesian Markov Chain Monte Carlo (MCMC). The calibrated system parameters are expressed by the posterior distributions rather than a point estimation. Results showed that Bayesian calibration outperforms the simulated annealing optimisation based calibration approach on model output biomass, and canopy cover results is along great agreement with biomass results avoiding overfitting problems. Therefore, Bayesian method provides one promising approach on crop model calibration reducing the uncertainties. In the future, the combination of multiple processed variables calibration will be considered rather than only one single variable like biomass or canopy cover. Furthermore, our work will also move to a field experiment and the observed data will be collected from UAVs and satellite remote sensing platforms. By integrating various sources observed data and the AquaCrop model, the Bayesian calibration results will improve further.

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