

## Photosynthetic parameter estimations by considering interactive effects of light, temperature and CO<sub>2</sub> concentration

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### Abstract

Biochemical leaf photosynthesis models are evaluated by laboratory results and have been widely used at field scale for quantification of plant production, biochemical cycles and land surface processes. It is a key issue to search for appropriate model structure and parameterization, which determine model uncertainty. A leaf photosynthesis model that couples the Farquhar-von Caemmerer-Berry (FvCB) formulation to four different leaf temperature models is used to investigate the photosynthetic characteristics across a range of temperature gradients using both light ( $A-Q$ ) and CO<sub>2</sub> response curves ( $A-C_i$ ). We used the Bayesian approach to fit the model to trial data of C<sub>3</sub> crop plants (soybean, wheat) in the North China Plain and estimated key photosynthetic parameters, such as the maximum carboxylation rate of Rubisco ( $V_{\text{cmax}25}$ ), the potential electron transport rate ( $J_{\text{max}25}$ ), leaf dark respiration in the light ( $R_{\text{d}25}$ ), mesophyll conductance ( $g_{\text{m}25}$ ) and the kinetic parameter of Rubisco ( $\Gamma^*_{25}$ ) at a reference temperature of 25 °C. The results showed that 1) the model with moderate complexity showed the best goodness of fit, while conversely the simpler and more complex models were under and over fitting with their corresponding data, respectively; 2) the non-peaked Arrhenius temperature response, which including both light and CO<sub>2</sub> responses data gave the best estimates for the key parameters among the four models; and 3) the temperature gradient used to verify the model has greatly improved the estimation of six key parameters ( $J_{\text{max}25}$ ,  $V_{\text{cmax}25}$ ,  $R_{\text{d}25}$ ,  $\Gamma^*_{25}$ ,  $K_{\text{c}25}$ ,  $g_{\text{m}25}$ ) with relatively more narrow confidence intervals (CIs) and showing regular

variation on temperature gradient. Overall, this method offers an accurate basis for estimating leaf photosynthesis parameters and may enhance the accuracy of canopy, ecosystem and even global vegetation models.

**Keywords:**  $A-Q$  curve;  $A-C_i$  curve; Arrhenius temperature equation; Leaf photosynthesis model; WinBUGS.

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**Abbreviations:**  $V_{\text{cmax}25}$ , maximum carboxylation rate of Rubisco;  $J_{\text{max}25}$ , potential electron transport rate;  $R_{\text{d}25}$ , dark leaf respiration in the light;  $g_{\text{m}25}$ , mesophyll conductance;  $I^*_{25}$ , the kinetic parameter of Rubisco;  $g_i$ , infinite  $\text{CO}_2$  transfer conductance;  $K_{\text{c}25}$  &  $K_{\text{o}25}$ , the Michaelis-Menten constant for  $\text{CO}_2$  and  $\text{O}_2$  binding by Rubisco;  $E(E_J, E_V, E_{\text{Gstar}}, E_{\text{gm}}, E_{\text{rd}}, E_{\text{kc}}, E_{\text{ko}})$ , activation energy parameters;  $H(H_J, H_V, H_{\text{gm}})$ , deactivation factor;  $\Delta S$  ( $\Delta S_J, \Delta S_V, \Delta S_{\text{gm}}$ ), entropy factor; AIC, Akaike's Information Criterion; BIC, Bayesian Information Criterion; CIs: confidence intervals.

## Introduction

Crop growth is constrained by many abiotic stresses, among which climatic conditions (solar radiation, rainfall and temperature) have significant impacts on crop production and are spatially variable (Roderick and Farquhar, 2002; Salazar-Gutierrez et al., 2013; Calama et al., 2013). In addition, increasing atmospheric  $\text{CO}_2$  concentrations may directly promote photosynthesis and decrease transpiration through the response of stomata to  $\text{CO}_2$  concentration (Medlyn et al., 2001; Yu et al., 2004), thereby decreasing soil water uptake and increasing water use efficiency (Lawlor and Mitchell, 1991; Parry et al., 2004; Hosaini et al., 2009). Canopy photosynthesis plays a key role in determining biomass accumulation and partitioning to leaves, stems, roots and storage organs. Many crop models such as APSIM use light use efficiency to calculate canopy photosynthesis (Timlin et al., 2006; Keating et al., 2003), which may be too simplified to capture interactive impacts of climate change and  $\text{CO}_2$  concentration on food production. Therefore, it is prospected to integrate biochemical photosynthesis modules into crop models for climate change impact assessment (Yu and Flerchinger, 2006).

Process-based photosynthesis models have received increasing attention due to their important role in quantifying ecosystem production and vegetation-climate interactions (Caemmerer, 2000; Oijen et al., 2005). One of the frequently used models is the Farquhar-von Caemmerer-Berry

(FvCB) photosynthetic model (Farquhar et al., 1980; Miao et al., 2009; Patrick et al., 2009; Zhu et al., 2011). FvCB model includes many parameters that cannot be directly measured. Fitting model against field leaf-gas exchange measurements to derive the values of key parameters is a normally used. Parameter estimation is a critical and complex issue and the goal of parameter estimation is to determine a set of parameter values to fit the model outputs to observed or trial data, so that parameterization can be viewed as an optimization issue or an inverse problem. Two methods exist, traditional optimization algorithms (e.g. ordinary least square regression, Gauss-Newton, steepest descent, the Levenberg-Marquardt algorithms) and modern intelligent methods (e.g. implementations of Bayesian statistics, genetic algorithms) (Malakoff, 1999; Patrick et al., 2009; Zhu et al., 2011). Statistical optimization methods commonly minimize an objective function such that best-estimate parameter values are obtained by reducing the sum of the square of residuals between observed and predicted data. In linear systems this method is more suitable, but in nonlinear systems (e.g. photosynthesis model), parameters are sensitive to initial conditions, suggesting the solutions may stabilize at 'local' optima rather than "global" optima (Miao et al., 2009). The number of identifiable parameters in process-based ecosystem model is low with traditional optimizing algorithms (Su et al., 2009). Bayesian approach has the potential to overcome these issues. It incorporates prior information to determine the likelihood that a given model can explain the measured data via a posterior function. Additionally, it provides a close approximation of the global solution with the mean and confidence intervals for each parameter (Barnard, 1958; Malakoff, 1999; Braswell et al., 2005). And the particular focus of this study is on how the data sources and models can be coupled within a Bayesian modeling framework.

Over the past few decades, fitting of photosynthetic CO<sub>2</sub> responses (e.g. an  $A-C_i$  curve) has been a common method for estimating leaf photosynthesis parameters under diverse conditions (Wullschleger, 1993; Idso et al., 1994; Caemmerer, 2000; Leuning, 2002; Manter and Kerrigan, 2004; Su et al., 2009; Zhu et al., 2010) in many plant physiology models (Harley et al., 1992). However, the choice of method to fit  $A-C_i$  curves has a substantial effect on the final value of key parameters, such as  $V_{cmax}$  (i.e., the maximum rates of carboxylation under Ribulose-1, 5-bisphosphate (RuBP) saturation),  $J_{max}$  (i.e., the potential light-saturated electron transport rate) and infinite CO<sub>2</sub> transfer conductance  $g_i$  (Ethier and Livingston, 2004).

Furthermore, incorporation of light response ( $A-Q$ ) data can improve the estimation of some key parameters (e.g., dark respiration  $R_d$ , the  $\text{CO}_2$  compensation point  $I^*$ , mesophyll conductance  $g_m$ ) (Yu et al., 2002; Patrick et al., 2009) and enhance estimation of parameters from  $A-C_i$  curves (e.g. the parameter  $J_{\max}$  is limited by  $C_i$ , irradiance and temperature). Although rarely incorporated into parameter estimation in leaf photosynthetic models, the integration of  $A-C_i$  and  $A-Q$  data could result in more credible posterior means and smaller confidence intervals (Patrick et al., 2009).

The interactions among light,  $\text{CO}_2$  and temperature in leaf photosynthesis models make it a challenging task to determine representative parameter values. The FvCB model has approximately 10 independent equations including about 20 parameters. Consequently, a Bayesian optimization approach is useful for model-data parsimony (Hu and Bentler, 1995; Mulaik et al., 1989). In this study, we used a Bayesian approach to fit parameters for photosynthesis in  $C_3$  crops (soybean and wheat) from  $A-Q$  and  $A-C_i$  curves using the revised FvCB biochemical-based model of leaf-level photosynthesis. The objectives of this paper are to (i) evaluate the Patrick model in irrigated crops, (ii) test the model structures with diverse complexities under a temperature acclimation gradient and (iii) identify the best model-data model to balance goodness of fit (high value of log-likelihood) against model complexity and estimate the key parameters of leaf photosynthesis at a standardized temperature 25 °C.

## Materials and Methods

### *Experiment*

This study was conducted at Yucheng Agricultural Experiment Station (36° 50' N, 116° 34' E, 28m a.s.l.), which is located in the North China Plain and affiliated with Chinese Ecosystem Research Network (CERN). Enough water and nutrients were applied in the croplands (Yu et al., 2002; Yu et al., 2004). Two types of  $C_3$  crops, wheat (*Triticum aestivum* cv. 39-118) and soybean (*Glycine max*) were sown in October 24<sup>th</sup> 2012 and April 15<sup>th</sup> 2013, respectively. The light and  $\text{CO}_2$  response curve data of wheat was measured on sunny days during 15-26 May 2013 and that of soybean was measured on 17-30 July 2013 and 29-31 May 2014. Thermal acclimation of photosynthesis was evaluated in soybeans during 29-31 May 2014.  $A-C_i$  and  $A-Q$  curves were measured at two saturation intensity levels (1400 and 2000  $\mu\text{mol m}^{-2} \text{s}^{-1}$ ) and four leaf temperatures (27, 30, 35 and 40 °C) (Figure 1).

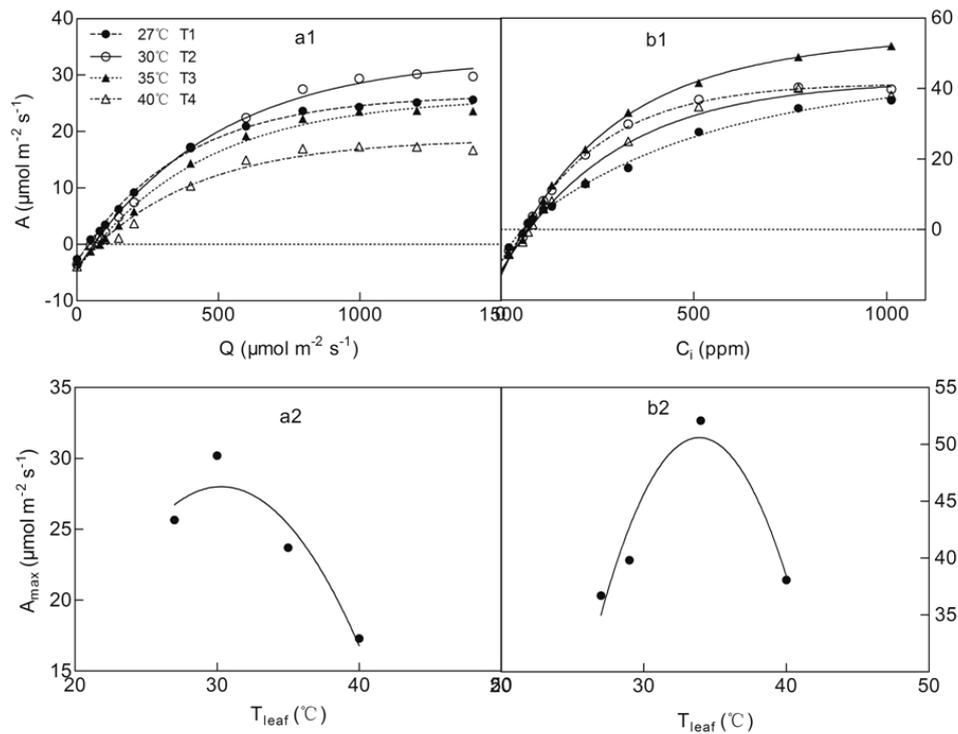


Figure 1. The light and CO<sub>2</sub> responses of photosynthesis (a<sub>1</sub>, a<sub>2</sub>) of soybean under different temperature and the changes in maximum photosynthetic rates with temperature (Yucheng, 29-31 May 2014).

Light and CO<sub>2</sub> response curves were measured on one leaf per seedling from 9:00 to 11:30 and 14:30 to 17:00 (total of 5 seedlings) using a Li-6400 portable photosynthesis system (Li-Cor, Lincoln, NE, USA). To reduce measurement errors, only the most recent fully expanded leaves were used. Each leaf was measured twice, first for  $A-Q$  and then for  $A-C_i$  curves. Relative humidity was kept at 60% and leaf temperature was maintained at initial levels throughout the measurement period (28-35 °C for wheat, 27-40 °C for soybean). Leaves were placed in a cuvette for 15 min to reach steady-state conditions for CO<sub>2</sub> exchange at light saturation ( $2000 \mu\text{mol m}^{-2} \text{s}^{-1}$ ) before measuring the  $A-C_i$  and  $A-Q$  curves. Intercellular CO<sub>2</sub> response curves were measured under saturated irradiance and at 10 increasing levels of CO<sub>2</sub> concentration (C<sub>i</sub>: 20, 60, 80, 120, 160, 200, 400, 600, 800 and 1000  $\mu\text{mol mol}^{-1}$ ). Light response curves were measured under an ambient CO<sub>2</sub>

concentration ( $380 \mu\text{mol mol}^{-1}$ ) and at 14 increasing levels of light intensity ( $Q$ : 0, 40, 60, 80, 100, 200, 600, 800, 1000, 1200, 1400, 1600, 1800 and  $2000 \mu\text{mol m}^{-2} \text{s}^{-1}$ ).

### Model Description

Measurements of  $\text{CO}_2$  assimilation rate ( $A_n$ ), intercellular  $\text{CO}_2$  pressure ( $C_i$ ), photosynthetic quantum flux density ( $Q$ ), leaf temperature ( $T_{\text{leaf}}$ ) and atmospheric pressure ( $P$ ) were used as driving variables to force the two models in this paper. We adopted the Bayesian model that proposed by Patrick et al. (2009) for the parameter optimization and uncertainty analysis of photosynthetic model, hereafter referred to as POT09. At the core of the model, a non-rectangular hyperbola was used for the FvCB biochemical model of photosynthesis in  $\text{C}_3$  plants (Ethier and Livingston, 2004). With a non-rectangular hyperbola, the additional curvature parameter  $\eta$  is related to the critical  $C_i$  ( $C_{\text{crit}}$ ) at which the function shifts from linear increase to flat (Gilmanov et al., 2003; Stoy et al., 2006), thereby representing the transition from limitation of photosynthesis by small  $C_i$  (e.g. the RuBP-saturated assimilation rate,  $A_c$ ) to limitation by regeneration of RuBP at large  $C_i$  (e.g. RuBP-limited net  $\text{CO}_2$  assimilation rate,  $A_j$ ) (Patrick et al., 2009).

In FvCB, photosynthesis is determined by the most limiting factor to assimilation rate:

$$A = \min \{A_c, A_j\} \quad (1)$$

where  $A_c$  is estimated when  $C_i < C_{\text{crit}}$  and  $A_j$  when  $C_i > C_{\text{crit}}$ . The list of equations used in the FvCB photosynthesis process model for determining  $A_c$  and  $A_j$  (Farquhar et al., 1980; Farquhar and Wong, 1984; von Caemmerer, 2000) were recently derived and compiled in Table 2 of Patrick et al. (2009). The limiting rate of photosynthesis, either  $A_c$  or  $A_j$ , is determined as a quadratic equation of three parameters, whose solutions are positive roots as following:

$$A_{c,j} = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \quad (2)$$

where  $a$  is the negative, inverse rate of mesophyll conductance in either case. The second and third parameters ( $b$ ,  $c$ ) represent processes that limit photosynthesis:

$$b = \frac{\tau - R_d}{g_m} + C_i + \phi \quad (3)$$

$$c = R_d(C_i + \phi) - \tau(C_i - \Gamma^*) \quad (4)$$

where the functions represented by  $\tau$  and  $\phi$  depend upon whether photosynthesis is limited by Rubisco activity ( $A_c$ ) or by electron transport ( $A_j$ ).

For calculation of  $A_c$ ,  $\tau$  is  $V_{cmax}$  and  $\phi$  represent the degree of photorespiration (i.e., uptake of  $O_2$  by Rubisco) as  $(1 + [O_2]) K_c/K_o$ , in which  $K_c$  and  $K_o$  are the Michaelis-Menten constants of RuBisCO for  $CO_2$  and  $O_2$ , respectively. To determine  $[O_2]$ , the partial pressure of  $O_2$  was assumed to remain 21 kPa. In  $A_j$ ,  $\tau$  is one-quarter of the rate of electron transport ( $J/4$ ) and  $\phi$  is  $2\Gamma^*$ . The rate of electron transport in FvCB is also determined as a quadratic function (McMurtrie et al., 1992; Patrick et al., 2009):

$$J = \frac{Q_{PSII} + J_{max} - \sqrt{(Q_{PSII} + J_{max})^2 - 4\theta Q_{PSII} J_{max}}}{2\theta} \quad (5)$$

where  $\theta$  is an empirical curvature factor (0.7; Evans, 1989) and  $Q_{PSII}$  is the fraction of photosynthetically active radiation ( $Q$ ) absorbed by PSII.  $Q_{PSII}$  is equal to  $\alpha (1 - f) Q / 2$ , where  $\alpha$  was set to 0.85 (von Caemmerer, 2000) and the spectral light quality factor  $f$  was set to 0.15 (Evans, 1987).

A central feature of POT09 is the temperature dependence of the photosynthetic parameter space  $\{K_c, K_o, \Gamma^*, g_m, R_d, V_{cmax}, J_{max}\}$  (Bjorkman et al., 1980; von Caemmerer, 2000). POT09 uses two temperature dependence schemes: peaked and non-peaked. The non-peaked function follows an Arrhenius exponential response to increasing temperature (Harley et al., 1992; Wullschleger, 1993). In all parameter estimations, temperature dependence was standardized to 25 °C (von Caemmerer, 2000; Leuning, 2002; Medlyn et al., 2002; Kattge and Knorr, 2007; Johnson et al., 1942; Harley et al., 1992; Zhu et al., 2010). Patrick et al. (2009) found that the peaked function, in which each parameter has an optimal temperature, above which parameter values again decline. For example,  $g_m$  increases exponentially with temperature to a peak within the range of 35 °C to 37.5 °C, above which  $g_m$  starts to decline (Bernacchi et al., 2002). Thus, POT09 uses a peaked temperature response function in addition to the Arrhenius

function by adding two parameters:  $H_\beta$  is the deactivation energy (i.e., the rate of decrease at temperatures above the optimum temperature) and  $\Delta S_\beta$  is an entropy factor.

Following POT09, we computed parameters for four FvCB photosynthesis models: two temperature response functions (non-peaked and peaked) and two data sources ( $A-C_i$  alone and  $A-C_i$  combined with  $A-Q$ ). Hereafter, implementations using data from only  $A-C_i$  curves will be denoted as models I and II for exponential and peaked temperature responses, respectively. Likewise, exponential and non-peaked temperature responses will be denoted as models III and IV, respectively, when referring to incorporation of data from both curves (Table 1).

Table 1. The statistic result for four model-data combinations.

Data		A- $C_i$		A- $C_i$ & A-Q	
		Non-peaked T	Peaked T	Non-Peaked T	Peaked T
Model		I	II	III	IV
Combination		I	II	III	IV
Model Validation	AICc	204.7	198.1	495.2	575.1
	R <sup>2</sup>	0.996	0.997	0.989	0.978

Notes:  $r^2$  values for observed versus predicted photosynthesis, obtained from the Bayesian model using A- $C_i$  data only and combined A- $C_i$  and A-Q data with either non-peaked or peaked temperature response functions for photosynthetic parameters.

### The Bayes approach

Parameter values were optimized in POT09 using a Bayes approach, which can be used to address multiple sources of variability present at different scales or levels (Kyveryga et al., 2013). In the Bayes approach, a probability distribution function (PDF) based upon prior information  $P(\beta)$  is combined if available with the probability of obtaining the data given the model parameters  $P(X|\beta)$ , to determine the probability of obtaining the model parameters given the data (i.e., the posterior probability  $P[\beta|X]$ ):

$$P(\beta|X) = P(\beta)P(X|\beta) \quad (6)$$

When no prior information is available, a non-informative  $P(\beta)$  can be assigned (e.g., multivariate normal). However, a large body of prior information exists in the photosynthesis literature (e.g., Michaelis-Menton and Arrhenius parameters; von Caemmerer, 2000; Patrick et al., 2009), thus  $P(\beta)$  can better constrain estimation of parameters.

Among the advantages of Bayesian in POT09, the data function  $P(X|\beta)$  is divided into two components: the observation function and the process equation based upon FvCB. The error ( $\sigma$ ) between measurements of photosynthesis and model predictions was assumed to be independent and normally distributed with mean zero:

$$P(X|\beta) = \frac{N}{\sqrt{2\pi\sigma}} \exp \left\{ -\sum_{i=1}^N \frac{(y_i - f[x_i|\beta])^2}{2\sigma^2} \right\} \quad (7)$$

where  $y_i$  is the observation and  $f(x_i|\beta)$  is the model prediction given the covariate  $x_i$  belonging to a set  $X$  of  $N$  observations and the parameter set  $\beta$ . Because  $P(\beta)$  and  $P(X|\beta)$  are multivariate normal and conjugates,  $P(\beta|X)$  is also normally distributed.

Bayesian analysis was performed using the Windows version of BUGS (Bayesian inference Using Gibbs Sampling, WinBUGS). WinBUGS is a fully extensible modular framework for constructing and analyzing Bayesian probability models that conducts the Bayesian analysis of complex statistical models through Markov-chain Monte-Carlo (MCMC) methods. The Metropolis-Hasting (MH) algorithm, a version of the MCMC technique, was adopted to generate a representative sample of parameter vectors from the posterior solution (Lunn et al., 2000; Yu and Meyer, 2006; Ntzoufras, 2009; Ke'ry, 2010). Following POT09, we set a burn-in period of 4000 iterations that were discarded from all summary statistics. Excluding burn-in samples, we tested 5,000, 10,000, 20,000 iterations to reduce the uncertainty of parameters and to infer the complexity of the parameter space.

#### *The model selection criteria*

"Information Criteria" provide an indication of the ability of a statistical model to fit a given dataset. Two such criteria are Akaike's Information Criterion (AIC) and the Bayesian Information Criterion (BIC), both of which integrate the number of unknown parameters and the complexity of the model space. AIC and BIC are more accurate when the number of

observations is large or the number of parameters ( $n$ ) is small, clearly as  $n$  increases, the BIC favors the simpler models with fewer parameters, which resulting in the AIC and BIC indices's disagree (Sotirios and Fernando, 2013). Therefore, a modified version of AIC with a correction for finite sample sizes (AICc) is preferred if the ratio of the number of observations to parameters is smaller than 40:1 (Burnham and Anderson, 2002), although AICc has a large penalty for extra parameters. In our study, the AICc between simulated and measured leaf photosynthesis rates was selected as an indicator of the calibration efficiency of the MCMC method.

The absolute value of AICc for a given model includes an arbitrary constant, thus an estimate of the absolute model fit is unobtainable. However, AICc is an effective metric for comparing the relative performance of two or more models. When comparing fitted objects, the smaller the AICc, the better the fit. For example, when the difference in AICc values between two models is larger than 10, the model with a worse fit can be removed from the selection process; a difference of 2 or less means models are roughly the same quality of fit (Burnham and Anderson, 2004; Yu and Meyer, 2006). The function of AICc is given as:

$$AIC_c = -2\log L + \frac{2(K+1)N}{N-K} \quad (8)$$

In the case of ordinary least squares regression or analysis of variance, the posterior likelihood ratio  $L$  can be calculated by the following equation,

$$\log(L) = -(N/2)\log(RSS/N) \quad (9)$$

Thus,

$$AIC_c = n \log(RSS/n) + 2N(K+1)/(N-K) \quad (10)$$

where  $RSS$  denotes the residual sum of squares from the fitted model and  $N$  and  $K$  are the number of observations and parameters, respectively. Moreover, as a rule of thumb, simulations were run until a specific tolerance was reached; in this case our tolerance was the Monte-Carlo error (MC error) less than 5% of the sample standard deviation (SD).

Table 2. Classification of posterior estimates for parameters in the photosynthetic model obtained from Bayesian method using the temperature modules and data combinations.

Parameter	□	□	□	□
$J_{\max 25}$	×	√	√	×
$V_{\text{cmax}25}$	×	√	√	√
$R_{d25}$	×	×	√	×
$\Gamma^*_{25}$	×	√	√	√
$g_{m25}$	×	×	√	×
$K_{c25}$	√	√	√	√
$K_{o25}$	-	-	-	×
$E_{\Gamma^*}$	-	-	-	×
$E_{Rd}$	-	-	-	×
$E_{kc}$	-	-	-	×
$E_{ko}$	-	-	-	×
$E_v$	-	-	-	×
$E_j$	-	-	-	×
$E_{gm}$	-	-	-	×
$H_g$	-	-	-	√
$H_j$	-	-	-	√
$H_v$	-	-	-	√
$\Delta S_g$	-	-	-	√
$\Delta S_j$	-	-	-	√
$\Delta S_v$	-	-	-	√

Notes: Combination I, II, III and IV are A-C<sub>i</sub> with non-peaked or peaked temperature functions, both data (A-C<sub>i</sub> combined with A-Q) with non or peaked temperature functions, respectively. Estimated parameters were well informed if the posterior estimates were in the range of prior CIs, showed regular variation on temperature gradient with relatively narrow CIs; poorly informed if the posterior estimates were similar to the prior means and had wide CIs; badly informed if the posterior estimates were out of the range of prior CIs with particularly large CIs. The signs √, -, × stand for well, moderately and poorly informed parameters, respectively.

## Results

### *Model and data selection*

Figure 2a shows a positive relationship between the computation time and the model complexity for all four iteration lengths. The time taken to reach convergence used by models I, II and III are close, (especially for models I and II) while model IV took longer time than the others (24000 iterations), approximately 4 times longer than model III. The values of AICc for the four models in their respective order are 204.7, 198.1, 495.2

and 575.1 (Table 1), although the differences in AICc between the models were relatively low, caution is still needed to verify that the MCMC method based on the Yucheng gas-exchange data can yield biologically significant estimations of parameters. The ratio of four models for eight key parameters shows that this criterion (MC error/SD) gives similar results comparing to AICc (Figure 2b): Neither model I nor IV appear as an inappropriate choice since both cannot give an effective estimation of key parameters (Table 2) and model IV costs too much time to calculate (Figure 2a). Additionally, both comparison of AICc and MC error/ SD among models informs us both under-fitting (model I) and over-fitting (model IV) were not the appropriate choice, it appears that only the moderate models (II and III) in this exercise are the most favorable candidates (see also Figure 4). Moreover, the ratio value of model II was very close to threshold value 0.05, while model III performed best, almost all parameters of it were far away from the threshold except only one value. Finally, model III was chosen as the most suitable model that incorporates temperature, light and CO<sub>2</sub> responses, while remaining parsimonious. Combined with the non-peaked T function and both  $A-C_i$  and  $A-Q$  data, model III gives the most reliable estimation values for these parameters (Table 2). High values of R<sup>2</sup> confirm that this coupled Bayesian photosynthetic model fit the data well for the bean and wheat; and prediction chart of model III shows that points in the plots of observed-versus-predicted photosynthetic rates fell tightly along the 1:1 line (Figure 3).

#### *The posterior distribution of photosynthetic parameters of model III*

The parameters of FvCB model were determined from random draws from the posterior solution for each model over successive iterations until convergence was reached. Discarding the burn-in period, summary statistics (mean and variance) were determined from binning the remaining chains to infer probability density functions (PDFs) for each estimated parameter. Below we outline the results relating to the posterior solutions of the parameter set used in model III.

In this study, the energy activation parameters ( $E$ ), the peaked temperature-response parameters of deactivation ( $H$ ) and entropy factor ( $\Delta S$ ) were poorly estimated; a consequence of constrained prior distributions (see Table 3). The main reason for this result is that these peaked parameters

( $H$  and  $\Delta S$ ) are not incorporated into the non-peaked Arrhenius temperature-response function, which can be estimated well only through light and  $\text{CO}_2$  curve data that itself has peaked temperature responses (Table 2 model IV).

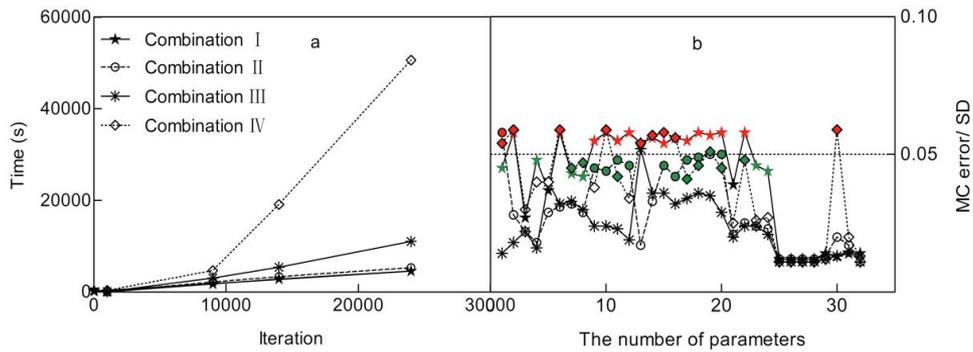


Figure 2. The four iterative calculations, 1000, 9000, 14000, 24000, respectively (a); the ratio (MC error / SD) of four combinations for eight key parameters (b). Note: red, green and black colors stand for the value is higher, close to and much lower than the threshold  $p$ -value 0.05, respectively.

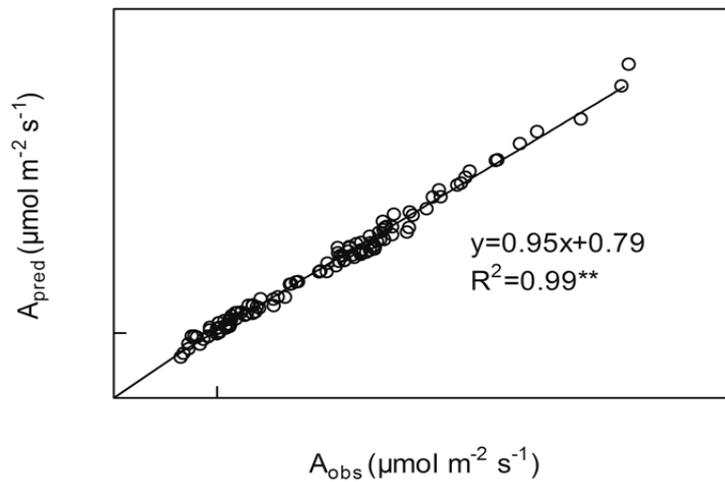


Figure 3. Comparison of measured ( $A_{\text{obs}}$ ) and model III predicted ( $A_{\text{pred}}$ ) values of  $\text{CO}_2$  assimilation. The parameter values are estimated from Bayesian optimization using both wheat and soybean data at Yucheng Agricultural Comprehensive Experiment Station during 15-26 May and 17-30 July 2013, respectively and  $**$  stands for 0.01 significance level.

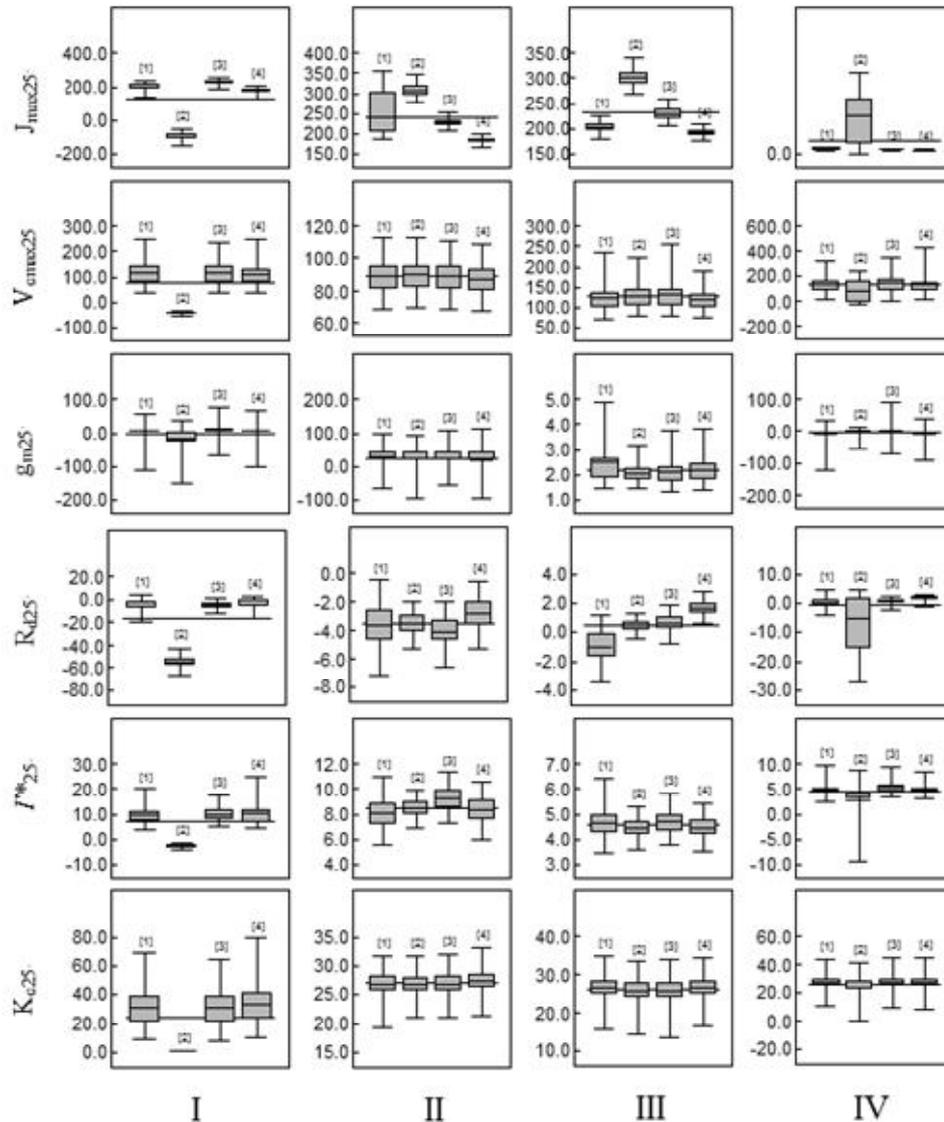


Figure 4. The boxplot of key parameters in 30,000 iterations of four temperature models (I, II, III, IV).

Note: The limits of each box represent the posterior quartiles, while the middle bars the posterior mean. The ending of the whisker lines represent the 2.5% and 97.5% posterior percentiles. While the horizontal reference line represents the posterior mean estimated from all nodes depicted in the plot. Additionally, 1.2.3.4 means different four data-sets.

Table 3. The posterior mean estimates and 95% CIs (i.e., 2.5<sup>th</sup> and 97.5<sup>th</sup> percentiles) for the key parameters of Model  $\beta$  of  $C_3$  plants.

Parameters	Median (95% CI)	Reference	Prior probability			Posterior probability		
			Bean1	Bean2	Wheat1	Wheat2		
$E_{V^*}$	26.8 (23.5,37.2)	Bernacchi et al. (2001), Ethier and Livingston (2004), Sharkey et al. (2007)	26.9 (24.1,29.6)	26.9 (23.9,30.0)	27.0 (24.1,29.9)	26.9 (24.1,29.7)		
$E_{Rd}$	63.9 (41.1,92.6)	Bernacchi et al. (2001), Ethier and Livingston (2004), Sharkey et al. (2007)	63.9 (61.1,66.7)	63.9 (61.0,66.6)	63.9 (61.0,66.7)	63.9 (61.1,66.7)		
$E_{Kc}$	80.0 (62.8,92.7)	Von Caemmerer (2000), Kosugi et al. (2003), Ethier and Livingston (2004), Sharkey et al. (2007)	70.4 (67.6,73.1)	70.3 (67.5,73.1)	70.3 (67.6,73.1)	70.3 (67.6,73.1)		
$E_{Ks}$	36.0 (18.5,37.8)	Von Caemmerer (2000), Kosugi et al. (2003), Ethier and Livingston (2004), Sharkey et al. (2007)	29.8 (27.1,32.6)	29.9 (27.1,32.7)	29.9 (27.1,32.6)	29.8 (27.0,32.6)		
$E_v$	65.4 (51.3,128.4)	Leuning (1997, 2002), Medlyn et al. (2002), Kattge and Knorr (2007), Sharkey et al.(2007), Patrick et al. (2009a)	65.5 (62.8,68.2)	65.5 (62.7,68.3)	65.5 (62.7,68.3)	65.5 (62.8,68.3)		
$E_j$	46.1 (35.9,105.6)	Leuning (1997, 2002), Medlyn et al.(2002), Kattge and Knorr (2007), Sharkey et al.(2007), Patrick et al. (2009a)	50.1 (47.3,52.9)	50.2 (47.1,53.2)	50.1 (47.0,53.2)	50.1 (47.3,53.1)		
$E_{gm}$	49.6 (n/a,n/a)	Sharkey et al.(2007)	49.6 (46.8,52.4)	49.6 (46.7,52.4)	49.6 (46.7,52.4)	49.6 (46.8,52.3)		
$H_g$	437.4 (n/a,n/a)	Sharkey et al.(2007)	437.4 (429,446)	437.4 (429,446)	437.4 (429,446)	437.4 (429,446)		
$H_j$	200 (130,214.7)	Leuning (1997, 2002), Medlyn et al.(2002), Kattge and Knorr (2007), Sharkey et al. (2007), Patrick et al. (2009a)	200 (191,208.8)	200 (191,208.7)	200 (191,208.8)	200 (191,208.8)		
$H_v$	200 (191,228.5)	Medlyn et al. (2002), Kattge and Knorr (2007)	200 (191,208.7)	200 (191,208.8)	200 (191,208.8)	200 (191,208.6)		
$\Delta S_g$	1.4 (n/a,n/a)	Sharkey et al. (2007)	1.4 (0.8,2.0)	1.4 (0.8,2.0)	1.399 (0.81,2.0)	1.399 (0.8,2.0)		
$\Delta S_j$	0.65(0.4,1.3)	Leuning (1997,2002), Medlyn et al. (2002), Kattge and Knorr (2007)	0.64 (0.4,0.9)	0.64 (0.4,0.9)	0.64 (0.4,0.9)	0.64 (0.4,0.9)		
$\Delta S_v$	0.65(0.4,1.3)	Leuning (1997,2002), Medlyn et al. (2002), Kattge and Knorr (2007)	0.65 (0.4,0.9)	0.65 (0.4,0.9)	0.65 (0.4,0.9)	0.65 (0.4,0.9)		

Notes: Median and 95% CIs for photosynthetic parameter values are derived from the literature; n/a indicates that information was not available in the literature.

The estimation results of remaining six key parameters of crop plants (bean and wheat) by model III gives the plots of posterior distribution of these parameters corresponding to the means and 95% CIs (i.e., 2.5<sup>th</sup> and 97.5<sup>th</sup> percentiles) (Figure 4). The posterior distribution indicated that the mean of all key parameters were updated well by MCMC procedure, but the posterior means of  $g_{m25}$  and the kinetic properties of RuBisCO ( $I^*_{25}$ ,  $K_{c25}$ ,  $K_{o25}$ ) standardized to 25 °C with relatively broad CIs (and thus of higher uncertainty) gave no big differences with the prior median. This demonstrated that these parameters were less identifiable under less informative priors and thus the posterior means of these four parameters can be held relatively constant for C<sub>3</sub> plants at a temperature of 25 °C. While the main photosynthetic parameters (e.g.,  $V_{cmax25}$ ,  $J_{max25}$  and  $R_{d25}$ ) had relatively narrow credible intervals, the posterior mean of  $V_{cmax25}$  for soybean and wheat ranged from 124.5 to 127.3 and from 118.8 to 131.4  $\mu\text{mol m}^{-2} \text{s}^{-1}$ .  $J_{max25}$  for soybean and wheat ranged from 202 to 301 and from 190.4 to 229.1  $\mu\text{mol m}^{-2} \text{s}^{-1}$ .  $R_{d25}$  for soybean and wheat ranged from -1.0 to 0.4 and from 0.6 to 1.7  $\mu\text{mol m}^{-2} \text{s}^{-1}$ , respectively.

#### *Model validation of Temperature gradient of model III*

We validated model III by testing it ‘out of sample’ along a temperature gradient using a separate, independent soybean dataset (from May 29 to 31, 2014). This temperature gradient had peak temperatures of a range, 27, 30, 35, 40 °C and light-saturation intensities of 1400  $\mu\text{mol m}^{-2} \text{s}^{-1}$  for the A-Q curves, CO<sub>2</sub>-saturation concentration of 1000  $\mu\text{mol m}^{-2} \text{s}^{-1}$  for the A-C<sub>i</sub> curves, respectively (Figure 1). Additionally, both A-Q and A-C<sub>i</sub> curves were measured along the same gradient but with different peak temperatures (see b<sub>1</sub> and b<sub>2</sub> in Figure 1), for instance, the peak photosynthetic rate of the A-C<sub>i</sub> curve was reached at a temperature of 35 °C and then followed by 30, 40 and 27 °C. The posterior PDFs of all parameters calculated by the Bayesian method are listed in Table 4. The only poorly informed parameters found here are those relating to activation energy, the peaked temperature parameters and  $K_{o25}$ . The estimation of the other six parameters are greatly improved with the inclusion of a temperature gradient, with an interesting shift in mean value and a narrowing of the CIs with a change in temperature (especially evident for  $V_{cmax25}$ ). With increasing temperature, the mean of  $R_{d25}$  increases while the means of  $I^*_{25}$  and  $g_{m25}$  decline. The values of  $V_{cmax25}$  and  $J_{max25}$  increase with temperature and reach a peak at 35 °C and then drop at 40 °C, which is exactly the opposite behavior seen with  $K_{c25}$ .

Table 4. The posterior distribution of photosynthetic parameters of the soybean data with temperature gradient (the mean and the range of parameter values between 2.5%-97.5% probability).

Parameters	Posterior probability		
	C <sub>i</sub> & Q (μmol m <sup>-2</sup> s <sup>-1</sup> )	C <sub>i</sub> =1000, Q=1400	C <sub>i</sub> =1400, Q=1000
T (°C)	27	30	35
E <sub>p</sub> <sup>*</sup>	26.88 (24.1, 29.7)	26.89 (24.08, 29.71)	26.85 (24.01, 29.69)
E <sub>pd</sub>	63.89 (61.14, 66.7)	63.88 (61.05, 66.65)	63.87 (61.05, 66.72)
E <sub>kc</sub>	70.38 (67.61, 73.14)	70.39 (67.59, 73.16)	70.26 (67.49, 73.05)
E <sub>so</sub>	29.83 (27.07, 32.59)	29.85 (27.04, 32.64)	29.89 (27.08, 32.64)
E <sub>v</sub>	65.48 (62.66, 68.32)	65.49 (62.73, 68.28)	65.61 (62.84, 68.4)
E <sub>j</sub>	50.1 (47.31, 52.89)	50.12 (47.35, 52.87)	50.14 (47.3, 53.03)
E <sub>gpm</sub>	49.6 (46.84, 52.37)	49.61 (46.82, 52.38)	49.62 (46.8, 52.46)
H <sub>g</sub>	437.4 (428.7, 446.2)	437.4 (428.6, 446.2)	437.4 (428.6, 446.1)
H <sub>v</sub>	200 (191.3, 208.8)	200 (191.2, 208.8)	200 (191.2, 208.8)
H <sub>t</sub>	200 (191.2, 208.8)	200 (191.3, 208.7)	200 (191.2, 208.7)
ΔS <sub>g</sub>	1.4 (0.78, 2.02)	1.4 (0.78, 2.01)	1.4 (0.78, 2.03)
ΔS <sub>v</sub>	0.65 (0.37, 0.93)	0.65 (0.37, 0.93)	0.65 (0.37, 0.93)
ΔS <sub>j</sub>	0.64 (0.36, 0.92)	0.64 (0.37, 0.92)	0.64 (0.36, 0.92)
J <sub>max25</sub>	188.6 (156.2, 228)	201.6 (170.6, 237.7)	238.1 (186.3, 287)
V <sub>emax25</sub>	88.34 (60.92, 115.2)	91.62 (66.47, 118.4)	95.51 (69.7, 132.1)
R <sub>0.25</sub>	-0.77 (-3.41, 1.5)	0.33 (-1.81, 2.23)	1.4 (0.16, 2.75)
I <sub>0.25</sub>	5.76 (3.64, 8.29)	4.79 (3.28, 6.63)	3.83 (2.71, 4.97)
g <sub>m0.25</sub>	1.78 (1.27, 2.73)	1.68 (1.21, 2.45)	1.28 (0.84, 1.99)
K <sub>e0.25</sub>	27.39 (20.39, 35.37)	26.55 (18.91, 33.02)	25.42 (15.38, 30.83)
K <sub>0.25</sub>	16600 (15970, 17230)	16600 (15970, 17220)	16600 (15970, 17230)

## Discussion

### *Maximum rate of electron transport $J_{max}$ and maximum carboxylation rate $V_{cmax}$*

The Bayesian method is able to derive the photosynthetic characteristic parameters for  $C_3$  crops using the diurnal  $CO_2$  gas-exchange and environmental temperature gradient data. This was especially evident with the two main parameters representing photosynthetic capacity,  $V_{cmax}$  and  $J_{max}$ . For example, regarding soybean,  $V_{cmax}$  varied from 88 ( $T=27\text{ }^\circ\text{C}$ ,  $Q=1400\text{ }\mu\text{mol m}^{-2}\text{ s}^{-1}$ ) to 134  $\mu\text{mol m}^{-2}\text{ s}^{-1}$  ( $T=31\text{ }^\circ\text{C}$ ,  $Q=2000\text{ }\mu\text{mol m}^{-2}\text{ s}^{-1}$ ) and for  $J_{max}$  values varied from 138 ( $T=40\text{ }^\circ\text{C}$ ,  $Q=1400\text{ }\mu\text{mol m}^{-2}\text{ s}^{-1}$ ) to 238  $\mu\text{mol m}^{-2}\text{ s}^{-1}$  ( $T=35\text{ }^\circ\text{C}$ ,  $Q=1400\text{ }\mu\text{mol m}^{-2}\text{ s}^{-1}$ ). However these values are dependent on the choice of the chosen temperature function. The posterior means of  $V_{cmax}$  and  $J_{max}$  determined for soybean and wheat are similar to these from Wullschleger (1993), especially for the soybean (*Glycine max*). When  $Q$  is  $1400\text{ }\mu\text{mol m}^{-2}\text{ s}^{-1}$ , corresponding  $V_{cmax}$  at a temperature of  $27\text{ }^\circ\text{C}$  is  $88\text{ }\mu\text{mol m}^{-2}\text{ s}^{-1}$ , very close to that of Harley and Sharkey (1991), but smaller than that of Parkhurst and Mott (1990). Additionally,  $J_{max}$  is a little larger than seen in other studies (Parkhurst and Mott, 1990; Harley and Sharkey, 1991) and is so for all other values determined from the temperature gradient. When  $Q$  reaches  $2,000\text{ }\mu\text{mol m}^{-2}\text{ s}^{-1}$ , the calculated values of both soybean (*Glycine max*) and wheat (*Triticum aestivum*) are similar to the estimates of soybean for  $J_{max}$  and  $V_{cmax}$  with 210 and 160  $\mu\text{mol m}^{-2}\text{ s}^{-1}$  (Pearcy et al., 1997), but they are generally larger than those values determined for  $Q < 2,000\text{ }\mu\text{mol m}^{-2}\text{ s}^{-1}$  (Table 5).

The posterior solution for photosynthetic parameter values were sensitive to different model structures (affecting the likelihood probability), plant types (affecting prior assumptions) and data-sets. Various functional responses have been used to describe the temperature dependence of  $V_{cmax}$  and  $J_{max}$ , such as exponential functions (Farquhar et al., 1980; Harley et al., 1992) and the third-order polynomials (Kirschbaum and Farquhar, 1984). The ratio of  $J_{max}$  and  $V_{cmax}$  is not constant with temperature, which varied from 1.97 to 2.68 (Kirschbaum and Farquhar, 1984) and has been further evidenced by Leuning (1997). Based on a non-peaked Arrhenius temperature function, the ratio of  $J_{max}$  and  $V_{cmax}$  varied from 1.36 to 2.5 in line with both of the above-mentioned studies (see Table 5).

Table 5. A comparison of  $V_{\text{cmax}}$  and  $J_{\text{max}}$  estimates of this study with previous research.

Species	Temperature (°C)	Irradiance ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ )	$V_{\text{cmax}}$ ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ )		$J_{\text{max}}$ ( $\mu\text{mol m}^{-2} \text{s}^{-1}$ )		Reference
			mean	95% CIs	mean	95% CIs	
Glycine max	25	900	94±2	88-99	168±1	167-170	Parkhurst and Mott, 1990
Glycine max	25	1500	83±9	53-112	160±4	109-211	Harley and Sharkey, 1991
Glycine max	27	1400	88	61-115	189	156-228	From this study
Glycine max	30	800	102±5	89-115	164±2	160-168	Harley et al., 1985
Glycine max	30	1400	92	67-118	202	171- 238	From this study
Glycine max	32	1700	48±5	27-69	132±10	105-157	Campbell et al., 1988
Glycine max	35	1400	96	70-132	238	186-329	From this study
Glycine max	40	1400	92	66-122	138	102-193	From this study
Glycine max	31	2000	134	76-251	229	205-257	From this study
Glycine max	36	2000	120	74-192	190	175-207	From this study
Glycine max	18	2000	126	70-240	201	180-227	From this study
Triticum aestivum	23	2000	130	78-226	301	268-341	From this study
Triticum aestivum	20	1000	57±2	53-61	130±1	127-133	Azcon-Bieto, 1983
Triticum aestivum	20	1500	67±1	62-72	189±6	115-263	Lawlor et al., 1989
Triticum aestivum	25	700	73±1	72-74	132±2	125-140	LeCain et al, 1989
Triticum aestivum	25	1000	83±5	67-99	193±2	189-197	Kriedem and Anderson, 1988

*Posterior distribution for parameters in the FvCB photosynthesis model*

Our posterior estimates for the activation energy, the Michaelis-Menten constant of Rubisco for O<sub>2</sub> and the temperature parameters were poorly informed by the photosynthetic data used, such that they were primarily constrained by the choice of prior distribution. Thus, eliciting prior valuable information distributions for the Bayesian method for these parameters is important to obtain correct estimations of the interested parameters (Tuyla et al., 2008; Patrick et al., 2009; Zhu et al., 2011). Furthermore, the values of these parameters cannot give an effective estimation solely through photosynthetic data. So that, these non-incorporate peaked temperature-response parameters and 'insignificant' energy activation parameters  $E$  (poorly estimated by four models, Table 2) could be considered as constant at standard 25 °C, reducing the degrees of freedom and simplifying the model, but this conclusion cannot simply apply to other temperature conditions. Given that certain parameters are invariant across the models, model complexity can be reduced by fixing these parameters, for example  $E_{Rd}$  at 63.9 KJ mol<sup>-1</sup>,  $H_v$  and  $H_l$  of 200,  $H_{gm}$  of 437.4 KJ mol<sup>-1</sup>,  $K_{025}$  of 16600 μmol mol<sup>-1</sup> (Leuning, 1997; Bernacchi et al., 2001; Leuning, 2002; Medlyn et al., 2002; Ethier and Livingston, 2004; Sharkey et al., 2007). These values agree with Von Caemmerer (2000), where such parameter values were generally fixed among higher C<sub>3</sub>, moreover, substantial controlled-condition experiments on interest species of these parameters are still needed in further studies to study their characteristics.

$R_{d25}$ , mitochondrial respiration standard to 25 °C, if assumed independent of light intensity and CO<sub>2</sub>, will lead to incorrect estimates of photosynthesis if carbon dioxide is being recycled within the leaf (Tenhunen et al., 1976). This bias of estimates may be attributed to the linear initial portion of carbon dioxide response curves due to mesophyll resistance to carbon dioxide transfer (Jones and Slatyer, 1972). Consequently, estimates of the magnitude of residual respiration were made by both  $A-Q$  and also several  $A-C_i$  curves to a point below zero net photosynthesis. Moreover, both Patrick et al. (2009) and Zhu et al. (2011) used a Bayesian approach to parameterize the same photosynthetic model and they confirmed that the addition of  $A-Q$  data with  $A-C_i$  data can give biologically viable estimates of  $R_{d25}$  as the diurnal course of  $Q$  improves the estimations. The parameter estimation using only  $A-C_i$  data may give negative value for the posterior mean for  $R_{d25}$ , which gives wider CIs and is slightly lower than the Bayesian

method (Von Caemmerer, 2000; Bernacchi et al., 2001; Dubois et al., 2007). The best estimates of the key parameters besides  $R_{d25}$  were from the method with both  $A-Q$  and  $A-C_i$  data, using non-peaked temperature response (Arrhenius) equation.

## Conclusion

The moderate complexity of the revised FvCB (Ethier and Livingston type) model with non-peaked Arrhenius temperature module is appropriate for the model-data fusion with two data sets ( $A-C_i$  data set or both  $A-C_i$  and  $A-Q$  data sets), while too simple or too complex model-data fusion are sub-optimal (leading to either under-fitting or over-fitting) for parameter estimation. Application of a temperature gradient to verify the model greatly improved our estimation of five key parameters ( $J_{\max 25}$ ,  $R_{d25}$ ,  $V_{c\max 25}$ ,  $I^*_{25}$ ,  $K_{c25}$ ,  $g_{m25}$ ). Posterior means of these parameters showed regular variation on temperature gradient with relatively more narrow CIs. However, inclusion of the temperature gradient data did not improve the estimation of  $K_{o25}$  and temperature parameters ( $E$ ,  $H$ ,  $S$ ). Therefore, it is advisable to use constant values of these parameters at standardized temperature 25 °C. Finally, we confirm that the Bayesian method coupled with  $A-Q$  curve data at different temperatures (like the diurnal or seasonal temperature variation) could be a good complement to the  $A-C_i$  curve fitting method to parameterize the photosynthetic model. These parameter values can be a measure of photosynthetic capacity and status of growth influenced by changing environment.

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