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# Optimization of water uptake and photosynthetic parameters in an ecosystem model using tower flux data



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### ABSTRACT

The soil water stress factor ( $f_w$ ) and the maximum photosynthetic carboxylation rate at 25 °C ( $V_{cmax}$ ) are two of the most important parameters for estimating evapotranspiration and carbon uptake of vegetation. Ecologically these two parameters have different temporal variations and thus their optimization in ecosystem models poses a challenge. To minimize the temporal scale effect, we propose a three-stage approach to optimize these two parameters using an ensemble Kalman filter (EnKF), based on observations of latent heat (LE) and gross primary productivity (GPP) fluxes at three flux tower sites in 2009. First, the EnKF is applied daily to obtain precursor estimates of  $V_{cmax}$  and  $f_w$ . Then,  $V_{cmax}$  is optimized at different time scales, assuming  $f_w$  is unchanged from the first step. The best temporal period is then determined by analyzing the coefficient of determination ( $R^2$ ) of GPP and LE between simulation and observation. Finally, the daily  $f_w$  value is optimized for rain-free days corresponding to the  $V_{cmax}$ curve from the best temporal period. We found that the variations of optimized  $f_w$  are largely explained by soil water content in the summer. In the spring, the optimized  $f_w$  shows a smooth increase following the rise of soil temperature, indicating that  $f_w$  may respond to the development of fine roots, which is related to the amount of accumulated heat in the soil. The optimized  $V_{\rm cmax}$  generally follows a pattern of a rapid increase at the leaf expansion stage in the spring, small variation in summer, and an abrupt decrease at foliage senescence. With eddy covariance fluxes data, data assimilation with a EnKF can retrieve the seasonal variations of water uptake and photosynthetic parameters in an ecosystem model, and such gives clues on how to model forest responses to water stress.

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## 1. Introduction

Terrestrial ecosystem models have been widely used to simulate carbon, water and energy fluxes and climate-ecosystem interactions (Dietze et al., 2011; Stoy et al., 2013). In these models, some vegetation and soil parameters are determined without consideration of their seasonal variations (Kattge et al., 2009). Data assimilation (DA) provides an effective way to optimize these parameters at different time scales (Kattge et al., 2009; Liu et al., 2012; Pauwels et al., 2007; Pipunic et al., 2008; Rayner, 2010; Wolf et al., 2006). Characterization of the seasonal variations of key ecosystem parameters is important in improving the performance of ecosystem models as the outcomes of the models generally respond to these parameters non-linearly (Wang et al., 2001).

The soil water stress factor  $(f_w)$  used in the stomatal conductance formulation and the maximum photosynthetic carboxylation rate at 25 °C ( $V_{cmax}$ ) are identified as two of the most important parameters related to the estimation of evapotranspiration and carbon uptake of vegetation (Ju et al., 2010; Mo et al., 2008; Wolf et al., 2006; Zhou et al., 2013 Zhu et al., 2009). The existing literature uses different seasonal patterns of these two parameters with different response to soil water depletion (Zhou et al., 2013):

(1) the soil water stress on photosynthesis has been implemented arguably either by adjusting  $V_{\text{cmax}}$  and/or  $J_{\text{max}}$  (maximum electron transport rate) (Cai and Dang, 2002; Dai et al., 2004;

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Grassi et al., 2005; Wang et al., 2007; Wang et al., 2001; Xu and Baldocchi, 2003), or modifying the slope of the Ball–Woodrow– Berry (BWB) equation (Arain et al., 2006; Bonan, 1995; Heroult et al., 2013; Ju et al., 2006; Wang and Leuning, 1998), or both (Ju et al., 2010; Keenan et al., 2009, 2010b; Reichstein et al., 2003);

- (2) a soil water stress factor  $f_w$  has been used to modify the original BWB equation (Ball et al., 1987) to include the important influence of soil water on stomatal conductance, but the mathematical form describing the influence differs in different studies. The form has been treated using linear (Arain et al., 2002; Bonan, 1995; Wang and Leuning, 1998; Wang et al., 2001), exponential, or power functions (Bonan, 1995; Ju et al., 2006). Various values of the slope of the BWB equation are reported (Heroult et al., 2013; Ju et al., 2010; Medlyn et al., 2011; Mo et al., 2008; Wolf et al., 2006).  $f_w$  was found to vary rapidly in response to soil water dynamics in the root zone (Vicente-Serrano et al., 2013).
- (3) the temporal variation of  $V_{\rm cmax}$  is often ignored or simply parameterized. In addition to its strong dependence on temperature (Medlyn et al., 2002), V<sub>cmax</sub> has been found to be linearly (Houborg et al., 2013; Kattge et al., 2009) or nonlinearly (Arain et al., 2006) related to leaf Rubisco-N (nitrogen). As the leaf N accumulates and depletes slowly through daily uptake and consumption in photosynthesis, we would not expect that the amount of Rubisco changes quickly on day-today basis (Yasumura et al., 2006). This intrinsic  $V_{cmax}$  can be inverted from the leaf photosynthesis measurement using Farguhar model (Farguhar et al., 1980) in optimal condition. Earlier studies suggested that DA of vegetation parameters at daily time steps leads to fast changing  $V_{\rm cmax}$  values that are unrealistic (Ju et al., 2010; Mo et al., 2008). This is because that the original Farguhar's model has no clear mechanism to describe how photosynthesis will change under stress conditions, such as the deactivation of Rubisco by extreme temperatures and soil water stress (Jensen, 2000), the breakdown of chlorophyll and the importance of mesophyll conductance (Keenan et al., 2010a). So a  $V_{cmax}$  inverted from the Farguhar's model under stress condition will have projected information from the missing model structures and apparently have larger temporal variations (Grassi and Magnani, 2005; Reichstein et al., 2003), and often is called "observed  $V_{cmax}$ " or "apparent  $V_{cmax}$ " (Zhou et al., 2013). The variations of apparent V<sub>cmax</sub> are modulated by slow variation of leaf N and variations of unexplained model structures (Keenan et al., 2010a).

In short, the temporal variations of these two parameters are in need of further investigation. In this study, we attempt to develop a new optimization scheme that can capture the temporal variation patterns of  $f_w$  and  $V_{cmax}$  based on measured water and carbon fluxes at three eddy covariance tower sites. Our objectives are: (1) to investigate how N-determined  $V_{cmax}$  varies seasonally in forest ecosystems; (2) to find the optimal time window, ranging from 1 day to 15 days, for determining  $V_{cmax}$  temporal variability; (3) to examine relationship between  $f_w$  and soil volumetric water content (VWC) in the root zone; and (4) to investigate if  $f_w$  is directly related to soil temperature when soil water is not the limiting factor in the early and late growth season.

## 2. Method and data

The boreal ecosystem productivity simulator (BEPS) ecosystem model (Chen et al., 1999, 2007, 2012) is used in this study. A full conceptual diagram of the model is described in Ju et al. (2006). It is a process-based ecosystem model that includes carbon, water, and energy budgets and soil thermal transfer modules. The gross primary productivity (GPP) is modeled by scaling Farquhar's leaf-level biochemical model (Farquhar et al., 1980) up to canopy-level using the "two-leaf" approach (Chen et al., 1999; Norman, 1982). The bulk stomatal conductance of the sunlit and shaded leaves for water vapor and  $CO_2$  is calculated using a modified BWB equation (Ball et al., 1987). The evaporation of intercepted water from the canopy and the ground surface is calculated using the Penman-Monteith equation (Monteith, 1965), and canopy transpiration from sunlit and shaded leaves is computed following Wang and Leuning (1998). The N-weighted  $V_{cmax}$  for sunlit and shaded leaves are obtained by taking account of the vertical profile of leaf N content and canopy structure (Chen et al., 2012). The BEPS model is described in detail below.

#### 2.1. Photosynthesis

The canopy-level photosynthesis ( $A_{canopy}$ ) is simulated as the sum of the total photosynthesis of sunlit and shaded leaf groups (Chen et al., 1999):

$$A_{\text{canopy}} = A_{\text{sun}} (g_{\text{sc, sun}}) L_{\text{sun}} + A_{\text{sh}} (g_{\text{sc, sh}}) L_{\text{sh}}$$
(1)

where the subscripts "sun" and "sh" denote the sunlit and shaded components of the photosynthesis (A) and leaf area index (LAI or L).  $g_{sc}$  is the stomatal resistance for carbon molecules. The sunlit and shaded LAI are separated by (Chen et al., 1999; Norman, 1982):

$$L_{\rm sun} = 2\cos\theta \left(1 - e^{-0.5\Omega L/\cos\theta}\right) \tag{2}$$

 $L_{\rm sh} = L - L_{\rm sun}$ 

where  $\theta$  is the solar zenith angle,  $\Omega$  is the clumping index and *L* is the leaf area index. The net rate of CO<sub>2</sub> assimilation (either sunlit or shaded parts) is calculated as (Farquhar et al., 1980):

$$A = \min(A_{\rm c}, A_{\rm j}) - R_{\rm d} \tag{3}$$

$$A_{\rm c} = V_{\rm cmax} f_V(T) \frac{C_{\rm i} - \Gamma}{C_{\rm i} + K_{\rm c}(1 + O_{\rm i}/K_{\rm o})} \tag{4}$$

$$A_{j} = J_{\max} f_{j}(T) \frac{C_{i} - \Gamma}{2(C_{i} - 2\Gamma)}$$
(5)

where  $A_{A_c}$ , and  $A_j$  are the net photosynthetic, Rubisco-limited and light-limited gross photosynthetic rates  $\mu$ mol m<sup>-2</sup> s<sup>-1</sup>, respectively.  $R_d$  is the daytime leaf dark respiration,  $V_{cmax}$  is the maximum carboxylation rate at 25 °C.  $J_{max}$  is the electron transport rate at 25 °C.  $C_i$  and  $O_i$  are the intercellular CO<sub>2</sub> and oxygen concentration, respectively.  $\Gamma$  is the CO<sub>2</sub> compensation point without dark respiration,  $K_c$  and  $K_o$  are the Michaelis–Menten constants for CO<sub>2</sub> and oxygen respectively.  $f_V(T)$  and  $f_j(T)$  are the air temperature (T) response function for  $V_{cmax}$  and  $J_{max}$  respectively. In the model, the  $J_{max}$  is estimated from  $V_{cmax}$  (Medlyn et al., 1999):

$$J_{\rm max} = 2.39 \times V_{\rm cmax} - 14.2 \tag{6}$$

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