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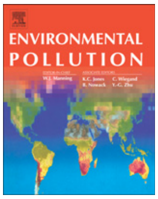

Analysis of a Farquhar-von Caemmerer-Berry leaf-level photosynthetic rate model for *Populus tremuloides* in the context of modeling and measurement limitations

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A photosynthetic rate model is parameterized for Populus tremuloides and evaluated based on its ability to predict dependent as well as independent data.

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ABSTRACT

The balance of mechanistic detail with mathematical simplicity contributes to the broad use of the Farquhar, von Caemmerer and Berry (FvCB) photosynthetic rate model. Here the FvCB model was coupled with a stomatal conductance model to form an [A,g_s] model, and parameterized for mature *Populus tremuloides* leaves under varying CO_2 and temperature levels. Data were selected to be within typical forest light, CO_2 and temperature ranges, reducing artifacts associated with data collected at extreme values. The error between model-predicted photosynthetic rate (*A*) and *A* data was measured in three ways and found to be up to three times greater for each of two independent data sets than for a base-line evaluation using parameterization data. The evaluation methods used here apply to comparisons of model validation results among data sets varying in number and distribution of data, as well as to performance comparisons of [A,g_s] models differing in internal-process components.

1. Introduction

The widely accepted, steady-state photosynthetic rate model of Farquhar, von Caemmerer and Berry (1980), the FvCB model, relates C_3 leaf gas exchange data to underlying limitations to photosynthesis at the leaf-tissue level due to the activity of Rubisco, regeneration of RuBP and stomatal conductance. The model achieves a useful balance between mechanistic detail and mathematical simplicity. Various modifications to the model have been developed in order to extend its responsiveness to a wide range of environmental conditions (Hikosaka et al., 2006; Rogers and Humphries, 2000) water and nutrient stress (Dewar, 2002; Kubiske et al., 2002), and elevated CO_2 and O_3 concentrations (Karnosky et al., 2003; Kull et al., 1996; Martin et al., 2000, 2001; Reich, 1983).

As noted by Farquhar, von Caemmerer and Berry (2001), the FvCB model does not include all mechanisms contributing to photosynthetic rate. Instead it represents an intelligent, simplified blend of processes occurring at the chloroplast level. Extrapolation of the model to the leaf-level, however, can result in erroneous assumptions about homogeneity of photosynthetic activity throughout the leaf, gas conductances and other internal processes (Flexas et al., 2008; Schurr et al., 2006). In order to predict photosynthetic rate from external rather than internal CO_2 concentration, the FvCB model is coupled with a stomatal conductance model, often of the Ball-Berry (Ball et al., 1987) or Leuning (Leuning, 1995) type, forming an [A,g_s] model.

Different strategies for calibrating the non-linear FvCB model, with its interdependent parameters, can lead to different sets of parameter values (see e.g. Sharkey et al., 2007). For example, Dubois et al. (2007) showed that, using standard parameterization methods, the assumed value of the A/C_i transition point alone can significantly influence the resulting estimates of V_{cmax}, J_{max} and R_d. (See the Appendix for symbol definitions and units.) Moreover, parameters for these components are typically determined as optimal regression fits to data and such fits can be sensitive to data distribution, inaccuracies and bias.

Unrecognized limitations and bias of instrumentation can also be misleading (Long and Bernacchi, 2003; Long et al., 1996). Estimates of respiration, CO_2 compensation point, V_{cmax} and J_{max} can all vary significantly with instrumentation and techniques

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(Bernacchi et al., 2002; Ethier and Livingston, 2004; Singsaas et al., 2003). Data collected at extreme C_a levels within a gas exchange chamber are proportionately more affected by measurement error, imprecision and CO_2 leakage and diffusion than when chamber C_a levels are close to external C_a levels (Long and Bernacchi, 2003; McDermitt et al., 1989; Rodeghiero et al., 2007). Because of the technique by which A is measured, CO_2 leaking or diffusing into the chamber at low chamber C_a reduces apparent A, while CO_2 leaking out of the chamber at high chamber C_a increases apparent A. Also the use of C_i in place of C_c introduces bias in estimation of V_{cmax} and J_{max} (Singsaas et al., 2003), though the difference between C_i and C_c is difficult to predict (Flexas et al., 2007, 2008).

Measurements to estimate J_{max} are often made at chamber $C_a = 2000$ ppm to ensure that CO_2 is saturating and hence photosynthesis is RuBP regeneration limited. However at very high cuvette C_a there can be measurement problems related to stomatal closure in illuminated leaves (Niinemets et al., 1999). Also, phosphate availability may curb RuBP regeneration (Niinemets et al., 1999; Sharkey, 1985), leading to underestimation of J_{max}.

This study parameterized and validated a coupled [A,g_s] model using leaf-level A/C_i data with the goal of predicting A at growth C_a levels while seeking to minimize measurement effects and unmodeled photosynthetic rate dynamics. Validation was based on the [A,g_s] model's predictions of measured A values for dependent (i.e. parameterization) and independent data sets. Parameterization and validation were limited to leaf-level photosynthetic rate for healthy, mature *P. tremuloides* Michx. sun leaves with environmental conditions typical of aspen forests, in the absence of water and nutrient stress.

2. Methods of model development

2.1. Mathematical model

In Farquhar et al. (1980) steady-state C_3 leaf photosynthetic carbon assimilation rate A is driven by intercepted light, CO_2, temperature, and humidity as well as internal leaf processes. Photosynthetic rate is assumed to be limited either by Rubisco-catalyzed carboxylation, the regeneration of RuBP controlled by electron transport rate, or the regeneration of RuBP controlled by the rate of triose-phosphate utilization, TPU. No evidence of TPU limitation was found in the data (Long and Bernacchi, 2003; von Caemmerer, 2000). Thus $A = \min\{A_c, A_j\}$, where Rubisco-limited A is given by

$$A_c = \frac{V_{c,max}(C_i - \Gamma^*)}{C_i + K_m} - R_d, \tag{1}$$

where $K_m = K_c(1 + \frac{O_i}{K_o})$, and RuBP regeneration limited A is given by

$$A_j = \frac{J(C_i - \Gamma^*)}{4.5C_i + 10.5\Gamma^*} - R_d \tag{2}$$

As in Harley and Tenhunen (1991), dark respiration was expressed as an Arrhenius function of temperature of the form

$$R_d = \exp(c)\exp(-\Delta H_a/(RT_k)) \tag{3}$$

The temperature dependencies for Γ^* and K_m were drawn from Bernacchi et al. (2002). The parameters V_{cmax} and J_{max} were modeled as in Harley and Tenhunen (1991), Harley et al. (1992b) and Medlyn et al. (2002) by peaked temperature functions of the form

$$P(T_k) = P_{opt}\left(\frac{\Delta H_d \exp\left(\frac{\Delta H_a(T_k - T_{opt})}{T_k R T_{opt}}\right)}{\Delta H_d - \Delta H_a\left(1 - \exp\left(\frac{\Delta H_d(T_k - T_{opt})}{T_k R T_{opt}}\right)\right)}\right), \tag{4}$$

where $P(T_k)$ is the value of the parameter at temperature T_k, P_{opt} is the maximum value of the parameter and T_{opt} is the temperature at which P_{opt} is achieved.

The rate of electron transport, J, was related to J_{max} according to

$$\Theta_{PSII}J^2 - (Q_2 + J_{max})J + Q_2 J_{max} = 0 \tag{5}$$

The temperature dependences of Θ_{PSII} and Q_2 were those of Bernacchi et al. (2003) for growth temperature 14 °C.

As implemented in LI-6400 (equations from Farquhar and Sharkey, 1982; and Farquhar and von Caemmerer, 1982),

$$C_i = \frac{(g_{tc} - E/2000)C_s - A}{g_{tc} + E/2000}, \tag{6}$$

for $C_s = \frac{F}{100S}C_r - A\Big/\frac{F}{100S} + 0.001E,$ where F is air flow rate and S is leaf surface area inside the cuvette. In this study, $g_{tc} = \left(\frac{1.6}{g_s} + \frac{1.37(0.5)}{1.42}\right)^{-1},$ where g_s has the form

$$g_s = \frac{a_1(A + R_d)}{C_i(1 + \frac{D_s}{D_o})} \tag{7}$$

This is a variation of the basic Ball-Berry-Leuning g_s model (Leuning, 1995).

2.2. Parameterization data

This study differs from previous work in the selection criteria developed and applied to data prior to parameterization. The intent was to use real-world data sets filtered to avoid or reduce uncertainty due to unmodeled photosynthesis dynamics associated with leaf-age, leaf-health, low stomatal conductance, photoinhibition, water stress or nutrient availability. The data were also filtered to reduce the effects of potential instrumentation-induced errors at very low or very high values of C_r. Model components were parameterized primarily to high-light data with C_r close to C_a growth levels, where steady-state photosynthesis measurements are most likely representative of photosynthesis in the field.

The data used for parameterization in this study were collected as part of the Aspen FACE project (Dickson et al., 2000; Karnosky et al., 2003), located at 45°30′ N, 89°30′ W. Leaf-level data were collected from *P. tremuloides* clone 216 growing in open-air conditions with exposure to elevated (550 ppm) and ambient (360 ppm) levels of CO_2 during the 1998 and 2000 growing seasons. All measurements were made using an LI-6400 portable open gas exchange photosynthesis system (LI-COR, 1998, 2006). Only data for leaves within a Leaf Plastochron Index (LPI) range of approximately 9–26 were used. This range includes predominately recently mature and mature leaves. Kull et al. (1996) placed leaf maturation, based on chlorophyll content, at about LPI 8, while Noormets et al. (2001a) placed leaf maturation at about LPI 11. Because photosynthetic rate capacity may diminish in over-mature leaves and in leaves damaged by ozone (Kim and Lieth, 2003; Reich, 1983; Schultz, 2003; Niinemets et al., 2005), data for clearly over-mature or damaged leaves were excluded according to LPI and cut-off values for A. For $Q \geq 1000$ μmol m^{-2} s^{-1}, A was required to be at least 15 μmol m^{-2} s^{-1} when $C_r > 300$ ppm and at least 20 when $C_r > 400$ ppm. Data for which measured g_s averaged less than 0.3 when C_i was between 145 and 500 ppm were also excluded as low g_s measurements could occur for various reasons associated with unmodeled leaf-tissue behavior (Farquhar and Sharkey, 1982; Leuning, 1995; Mott and Buckley, 2000; Noormets et al., 2001b).

The full parameterization data set, the [A,g_s]-data, was the union of the first three limited data sets listed in Table 1. A large proportion of the [A,g_s]-data were for C_r levels between 340 and 560 ppm, since predicting A for ambient growth conditions was of highest priority. All of the data for $C_r < 400$ ppm was for leaves grown at day-time C_a close to 350 ppm and all of the data for $C_r > 400$ ppm was for leaves grown under elevated day-time C_a, about 550 ppm. The A_c-data consisted of the FACE-1998$_A$ data for which $C_r \leq 360$ ppm and the FACE-1998$_B$ data for which A appeared to be RuBP carboxylation-limited based on A/C_i curves. The A_j-data comprised the low-light FACE-2000 data, the FACE-1998$_A$ data for which C_r was above 540 ppm and the FACE-1998$_B$ data for which C_i was at or above the cross-over point.

The V_{cmax} parameterization data set (V-data) consisted of the A_c-data for which C_r was approximately 250–530 ppm. This included FACE-1998$_A$ data for C_r between 340 and 360 ppm and FACE-1998$_B$ A/C_i data for which C_i was nearly as high as the apparent transition point or the next C_i measurement below that. These values of C_i increased with temperature.

Table 1

Parameterization and validation data sets, with external variable ranges.

Name	R_d measured	C_a ppm	Q μmol m^{-2} s^{-1}	Temp °C	RH %	Reference
Parameterization data sets						
FACE-1998$_A$	no	360, 550	1000–1500	24–36	42–75	Noormets et al., 2001a
FACE-2000	no	1500	0–500	21–29	58–77	Noormets et al., 2010
FACE-1998$_B$	yes	50–410	1000–1500	19–36	23–81	
Validation data sets						
BOREAS TE-12	yes	70–400	0–2100	15–37	15–33	Arkebauer, 1998
FACE-1999	no	360, 560	1188–1300	17–35	46–77	Noormets et al., 2001b