Evaluating the CROPGRO–Soybean Model Ability to Simulate Photosynthesis Response to Carbon Dioxide Levels

G. Alagarswamy,* K. J. Boote, L. H. Allen, Jr., and J. W. Jones

ABSTRACT

Atmospheric carbon dioxide concentration $[CO_2]$ will increase in the future and will affect global climate and ecosystem productivity. Crop models used in past assessments of climate change effect on ecosystem productivity have not been adequately tested for the ability to simulate ecosystem responses to $[CO_2]$. Our objective was to evaluate the ability of the default CROPGRO–Soybean model to predict the responses of net leaf photosynthesis (A) and canopy photosynthesis (A_{can}) to photosynthetic photon flux (PPF) at different $[CO_2]$. We also compared the default leaf photosynthesis equations in CROPGRO with the full Farquhar equations for ability to predict the response of A to $[CO_2]$. Simulated and observed A and A_{can} were light saturated at 800 μmol m^{-2} s^{-1} PPF at ambient $[CO_2]$ but did not light saturate at PPF >1100 μmol m^{-2} s^{-1} at elevated $[CO_2]$. Observed and simulated A responded asymptotically to increasing intercellular $[CO_2]$. The CROPGRO default photosynthesis equations and the Farquhar equations simulated A equally well at all $[CO_2]$. Doubled $[CO_2]$ increased simulated A by 52% and A_{can} by 42%; these values are close to the increases of 39 to 48% for A and 59% for A_{can} reported in the literature. Root mean square errors for simulated A and A_{can} were low, and Willmott's index of agreement ranged from 0.86 to 0.99, confirming that the CROPGRO model with default photosynthesis equations can be used to evaluate potential effects of $[CO_2]$ on soybean photosynthesis and productivity.

INCREASE of carbon dioxide concentration $[CO_2]$ in the atmosphere will change future global climate via increased temperature and altered precipitation patterns, which affect ecosystem productivity. Carbon dioxide concentration steadily increased from 280 μmol CO_2 mol^{-1} during the preindustrial period (around the year 1750) to about 375 μmol CO_2 mol^{-1} in the year 2000. Projections of $[CO_2]$ in the year 2100 will range from 540 to 970 μmol CO_2 mol^{-1} of air, depending on emission scenarios (Houghton et al., 2001). The projected rise in $[CO_2]$ will influence plant processes at various hierarchic levels from short-term effects on net leaf photosynthesis (A) to long-term effects on primary productivity of terrestrial ecosystems.

Approaches to predict the effects of climate change on primary productivity often involve the use of mechanistic ecosystem simulation models coupled to climate change predictions from atmospheric general circulation models. Crop simulation models have been used to assess the productivity responses of various crops to anticipated future changes in $[CO_2]$ and temperature (Adams et al., 1990; Wang et al., 1992; Easterling et al., 1993; Wall et al., 1994; Matthews et al., 1995). Using the SOYGRO model V5.42 (Jones et al., 1989) with empiric adjustments to simulate effects of $[CO_2]$ on biomass accumulation, Peart et al. (1989) evaluated the impact of $[CO_2]$ on potential soybean production. The CROPGRO model (Boote et al., 1998) is more mechanistic than the SOYGRO model. Leaf photosynthesis simulation in CROPGRO is an adaptation of the equations of Farquhar et al. (1980) in an hourly leaf-level to canopy assimilation scaling approach with hedge-row light interception. The goal of this paper is to evaluate the CROPGRO model for its ability to simulate soybean leaf and canopy assimilation response to $[CO_2]$.

The leaf photosynthesis model of Farquhar et al. (1980) has been widely used to simulate response of A to $[CO_2]$. This model assumes that A is limited by the slower of two processes, namely the maximum rate of Rubisco-catalyzed carboxylation (Rubisco-limited) and the Ribulose 1,5 bisphosphate (RuBP) regeneration rate controlled by electron transport rate (RuBP-limited). The Farquhar model requires Rubisco enzyme kinetic parameters. Some of the kinetic parameters of the Rubisco enzyme, such as Michaelis constants for oxygen (K_o) and for CO_2 (K_c) and CO_2 compensation point in the absence of dark respiration ($\Gamma*$), are constant across species of C_3 plants. However, other required parameters that depend on the Rubisco enzyme concentration, such as maximum RuBP-saturated rate of carboxylation ($V_{c,max}$), maximum RuBP-saturated rate of oxygenation ($V_{o,max}$), and dark respiration rate (R_d), vary even within individual plants because they are conditioned by growing conditions. This makes application of the Farquhar model in mechanistic crop simulation models difficult.

The CROPGRO model uses a modified Farquhar and von Caemmerer (1982) approach in which only the RuBP-limited part is used to simulate responses of A to $[CO_2]$. Unlike the leaf photosynthesis model of Farquhar et al. (1980) and Farquhar and von Caemmerer (1982), CROPGRO's default leaf photosynthesis equations do not require K_c, K_o, $V_{c,max}$, or the maximum rate of electron transport (J_{max}) to simulate A. Rather, the approach in CROPGRO defines light-saturated leaf photosynthetic rate (A_{max}) at reference values of CO_2, O_2, temperature, reference specific leaf weight (SLW-REF), and leaf nitrogen (N) concentration. It uses an

G. Alagarswamy and K.J. Boote, Dep. of Agronomy, Univ. of Florida, Gainesville, FL 32611-0500; L.H. Allen, Jr., USDA-ARS and Dep. of Agronomy, Univ. of Florida, Gainesville, FL 32611-0965; and J.W. Jones, Dep. of Agricultural and Biological Engineering, Univ. of Florida, Gainesville, FL 32611-0570. Florida Agric. Exp. Stn. Journal Ser. no. R-10598. Received 6 Dec. 2004. *Corresponding author (alagarsw@msu.edu).

Abbreviations: LAI, leaf area index; MSE, mean squared error; MSE$_s$, systematic mean squared error; MSE$_u$, unsystematic mean squared error; PPF, photosynthetic photon flux; QE, quantum efficiency; RuBP, ribulose 1,5 bisphosphate; RMSE, root mean squared error.

Table 1. Experimental protocols for growing plants and measuring CO_2 assimilation rate in various data sets used in the model evaluation.

Data source	Pot size	Plant age at A† measurement	Growth CO_2 level	Light level		Temp.	
				Growth PPF	Measurement PPF	For growth (day/night)	For A measurement
		d	$\mu mol\ mol^{-1}$	$\mu mol\ m^{-2}\ s^{-1}$		°C	
Valle et al. (1985)	2000 L‡	72	350	natural§	0–1130	31/23	32
Harley et al. (1985)	12.5 cm diam.	23	350	800	>2000	30/20	30
Harley et al. (1985)	12.5 cm diam.	23	350	800	800	30/20	30
Campbell et al. (1990)	2000 L‡	34	160–990	natural¶	0–1370	31/23	30–33
Sims et al. (1998)	8 L	42–56	350	1300	1500	28/22	28
Griffin and Luo (1999)	5 L	24	350, 700	1300	1500	28/20	25

† A, net leaf photosynthesis; PPF, photosynthetic photon flux.
‡ Soybean plant community rooting volume was 66 L plant^{-1}.
§ PPF varied diurnally from 0 to 1130 $\mu mol\ m^{-2}\ s^{-1}$ during growth.
¶ PPF varied diurnally from 0 to 1350 $\mu mol\ m^{-2}\ s^{-1}$ during growth.

asymptotic exponential light response equation to simulate A, where quantum efficiency (QE) and A_{max} are dependent on $[CO_2]$, O_2, and temperature (Boote and Pickering, 1994). Models of photosynthesis at a canopy ecosystem level require not only equations describing CO_2 fluxes at leaf level but also some method of scaling photosynthesis from leaf to canopy level. CROPGRO simulates hourly A_{can} using a hedge-row light interception model and leaf-level photosynthesis parameters (Boote and Pickering 1994; Pickering et al., 1995). Briefly, the model computes absorption of direct and diffuse irradiance by sunlit and shaded leaf classes as a function of canopy height, width, leaf area index (LAI), leaf angle, row direction, latitude, day of year, and time of day. The A_{can} is the sum of sunlit and shaded leaf photosynthetic rates over their respective LAI classes.

Before applying the CROPGRO model in future assessments of climate change effects, its ability to predict $[CO_2]$ effects on A and A_{can} should be evaluated using results from controlled-environment studies. Our objectives were to evaluate the CROPGRO–Soybean model for predictions of (i) response of A to PPF at 330 (ambient) and 660 (elevated) $\mu mol\ CO_2\ mol^{-1}$, (ii) response of A to sub- to supra-ambient $[CO_2]$, (iii) response of A_{can} to PPF at sub- and supra-ambient $[CO_2]$, and (iv) to compare the simulation of A response to intercellular $[CO_2]$ (C_i) with CROPGRO's default photosynthesis equations compared with the full Farquhar equations. To evaluate model performance, we followed the statistical model testing procedures of Willmott (1981) and Willmott et al. (1985).

MATERIALS AND METHODS
Description of Data Sets Used in Model Evaluation

Data published by Valle et al. (1985) were used to test the simulated response of A to PPF at ambient and elevated $[CO_2]$. Data published by Harley et al. (1985), Valle et al. (1985), Sims et al. (1998), and Griffin and Luo (1999) were used to test the model's ability to simulate the response of A to C_i. We used A_{can} data of Campbell et al. (1990) for soybean canopies grown at six sub- to supra-ambient $[CO_2]$ to simulate A_{can} response to PPF. The experimental protocols describing growth conditions, age of plants, and photosynthesis measurement conditions are given in Table 1. Data from Harley et al. (1985) contained two sets of experiments. In one of the experiments, the light levels during A measurements were high (PPF > 2000 $\mu mol\ m^{-2}\ s^{-1}$) compared with growth-light level, and we designated this experiment as a high-light

experiment. In another experiment, the light level during A measurement was low and same as growth intensity (PPF = 800 $\mu mol\ m^{-2}\ s^{-1}$), and we designated this as a low-light experiment.

Net Leaf Photosynthesis Simulation

For these simulations, we used the default unmodified code and equations of the CROPGRO model (V4.0), where A is simulated using an asymptotic exponential light-response equation:

$$A = A_{max} \times [1.0 - \exp(-QE \times PPF/A_{max})] \quad [1]$$

where A is the net rate of CO_2 uptake per unit leaf area ($\mu mol\ m^{-2}\ s^{-1}$), A_{max} is the light-saturated A (defined at 30°C, 350 $\mu mol\ CO_2\ mol^{-1}$, 21% O_2, leaf nitrogen [N] concentration of 55 g kg^{-1}, and SLWREF of 35.0 g m^{-2} leaf area); and QE is the quantum efficiency of the leaf, which is referenced at the same conditions. Beginning with the 1994 release of the CROPGRO model, temperature and CO_2 effects on QE and A_{max} have been modeled using a modification of the Farquhar and von Caemmerer (1982) method as described in Eq. [37], [38], and [41] of Boote and Pickering (1994) and as described by Pickering et al. (1995). For simulating A, we used the following default soybean model input parameters: A_{max} = 1.00 mg CO_2 m^{-2} s^{-1} (22.7 $\mu mol\ CO_2$ m^{-2} s^{-1}) defined at SLWREF = 35.0 g m^{-2}, and leaf nitrogen (N) concentration = 55 g kg^{-1}. Specific leaf weight (SLW) and leaf N concentration normally vary during model simulations due to climatic and management conditions. Thus, actual single-leaf A_{max} was modeled as a linear function of SLW and as a quadratic function of leaf N concentration. The rationale for the effect of SLW on A_{max} was that thick leaves have more chloroplasts and a higher mass of photosynthetic enzymes and thereby have enhanced photosynthetic capacity per unit leaf area. Hence, SLW and leaf N concentration were model state variables that influenced A_{max}. To simulate the leaf conditions for the specific days of tested experiments, we input into the model the SLW, leaf N concentration, LAI, hourly PPF, temperature, and $[CO_2]$ for any day and output the hourly means of instantaneous gross A and A_{can}. The SLW data for the Valle et al. (1985) data set were taken from a comparable study by Allen et al. (1988). The SLW data were not available from Harley et al. (1985) but were derived by running the crop model for the growth temperature and PPF conditions up to the specific day when photosynthesis was measured. The SLW and leaf N inputs for testing simulations of Sims et al. (1998) were taken from a comparable study by Luo et al. (1998), and SLW and leaf N data for testing simulations of Griffin and Luo (1999) were taken from the study by Griffin and Luo (1999).

Dark Respiration Rate

The CROPGRO model simulates gross leaf A and A_{can} and separately computes growth and maintenance respiration of each tissue type. Thus, the model does not normally compute net A. However, to compare with published data on net A, we took the outputs of simulated gross A and subtracted the observed R_d. Sims et al. (1998) and Griffin and Luo (1999) measured net A and R_d. Harley et al. (1985) measured R_d as a function of leaf temperatures (TLEAF) varying from 15 to 45°C. We fitted a nonlinear relationship to the data.

$$R_d = 0.0117 \times \text{TLEAF}^{1.59}$$

$$r^2 = 0.97 \qquad [2]$$

For the Harley et al. (1985) data, simulated net A was derived by subtracting R_d calculated with Eq. [2] from the modeled gross photosynthesis. For the Valle et al. (1985) data, R_d values for ambient and elevated $[CO_2]$ were obtained from graphs as the y intercept where the PPF was zero. For the Campbell et al. (1990) data, we used the modeled total canopy respiration (including growth and maintenance components) for the specific day when A_{can} was measured. Total modeled respiration was interpolated for the observed temperature using canopy R_d and air temperature relationships developed by Pan (1996). Net A_{can} was derived by subtracting the interpolated R_d from modeled gross A_{can}.

Comparison of CROPGRO's Default Photosynthesis Equations with Farquhar Photosynthesis Equations

We compared CROPGRO's default photosynthesis equations with the full Farquhar equations for their ability to predict A response to C_i. We used A vs. C_i (A/C_i) data published by Sims et al. (1998), Griffin and Luo (1999), and Harley et al. (1985) for model comparison. The parameters K_c, K_o, $V_{c,max}$, J_{max}, and R_d required for the Farquhar equations were taken from these publications. The $V_{c,max}$ values were 48.7 and 49.2 μmol m^{-2} s^{-1} for soybean grown at ambient and elevated $[CO_2]$, respectively, in the Griffin and Luo (1999) data set and 83.6 μmol m^{-2} s^{-1} for the Sims et al. (1998) data set. The J_{max} values were 131.3 and 139.6 μmol m^{-2} s^{-1} for soybean grown at ambient and elevated CO_2, respectively, in the Griffin and Luo (1999) data set and 184.8 μmol m^{-2} s^{-1} for soybean in the Sims et al. (1998) data set.

Evaluation of Model Performance

We compared simulated and observed A and A_{can} using a linear regression approach in conjunction with the deviation-based statistical measures and dimensionless index of agreement (D) as suggested by Willmott (1981) and Willmott et al. (1985). In this method, we used observed and simulated A in response to various levels of PPF and C_i and hourly mean values of observed and simulated A_{can} (from 0700 to 1700 h). The deviation-based statistical parameters (root mean squared error [RMSE] and its systematic [RMSE$_s$] and unsystematic [RMSE$_u$] components and Willmott's index of agreement [D index]) were used to compare how well modeled A and A_{can} compared with the observed values. Because there was no calibration of the model, the results reported in this study can be considered a validation of model performance in predicting A and A_{can}.
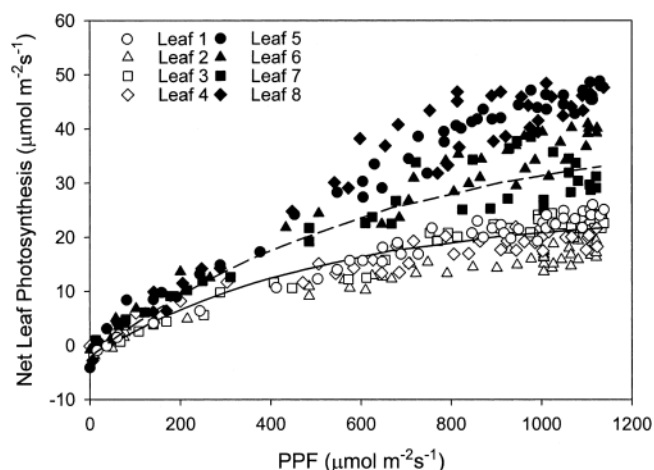

Fig. 1. Simulated soybean net leaf photosynthesis (A) response to PPF. Symbols are for measured data for eight different leaflets (adapted from Valle et al., 1985), and curves are for simulations using default CROPGRO photosynthetic equations. Open symbols and solid line are for ambient $[CO_2]$ (330 μmol mol^{-1}); solid symbols and dashed line are for elevated $[CO_2]$ (660 μmol mol^{-1}).

RESULTS AND DISCUSSION

Response of Net Leaf Photosynthesis to Photosynthetic Photon Flux at Ambient and Elevated Carbon Dioxide Concentration

The rate of regeneration of CO_2 acceptor RuBP is dependent on the concentrations of the high-energy nucleotides ATP and reduced NADPH, both of which depend on photochemical energy supply and rates of whole-chain electron transport. Thus, it was essential to evaluate the model capability to simulate the response of A to photochemical energy supply, which is controlled by PPF. Observed and simulated A increased as PPF increased and were light saturated at 800 μmol m^{-2} s^{-1} PPF at ambient $[CO_2]$ (330 μmol mol^{-1}). At high light (PPF > 1100 μmol m^{-2} s^{-1}), simulated A was 21.7 μmol m^{-2} s^{-1}, closely matching the observed A of 21.4 ± 3.1 μmol m^{-2} s^{-1} (mean ± SD of four leaves) (Fig. 1). At elevated $[CO_2]$ (660 μmol mol^{-1}), simulated A was 33.1 μmol m^{-2} s^{-1}, but the observed A was 41.4 ± 8.4 μmol m^{-2} s^{-1} (mean ± SD of four leaves), indicating that model underpredicted observed A. Grant (1989, 1992) had previously used data from Valle et al. (1985) to test a leaf photosynthesis model that contained the full Farquhar and von Caemmerer (1982) leaf photosynthesis equations. Grant (1989) tested the response of A to irradiance and showed that the simulated light-response curves closely matched the observed curve of Valle et al. (1985) at ambient $[CO_2]$, whereas the model underpredicted the response of A to irradiance at elevated $[CO_2]$ above 400 μmol m^{-2} s^{-1} PPF. Grant's model underpredicted A by 24% at PPF >1100 μmol m^{-2} s^{-1}. In a second paper, Grant (1992) again showed that the leaf photosynthesis model underpredicted A by 14% at elevated $[CO_2]$ compared with the data of Valle et al. (1985). The CROPGRO model simulations of response of A to PPF were similar to the results reported by Grant (1989, 1992). Our results, taken together with Grant's simulations, indicate that it is likely that the

Table 2. Mean ± SD of net leaf photosynthesis and results of regression analysis $P_i = a \times O_i + b$, where O_i are observed (Valle et al., 1985) and P_i are simulated leaf photosynthesis by the default CROPGRO equations for two $[CO_2]$. Also shown are Willmott's index of agreement, root mean square error, and the systematic and unsystematic components of the root mean square error.

[CO₂]	N	A† (mean ± SD)‡		Slope (a)	SE_a	Intercept (b)	SE_b	r²	D	RMSE	RMSE_s	RMSE_u
		Observed	Simulated									
μmol mol⁻¹		μmol m⁻² s⁻¹								μmol m⁻² s⁻¹		
330	10	15.2 ± 6.70	16.0 ± 6.83	0.95	0.121	1.50	1.990	0.89	0.97	2.34	0.86	2.18
660	11	27.1 ± 14.95	21.5 ± 12.50	0.82	0.064	−0.63	1.967	0.95	0.93	6.85	6.28	2.74

† A, net leaf photosynthesis; D, Willmott's index of agreement; RMSE, root mean square error; RMSE_s, systematic component of the root mean square error; RMSE_u, unsystematic component of the root mean square error; SE_a, standard error for slope; SE_b, Standard error for intercept.
‡ Mean ± SD of observed (O_i) and simulated (P_i) hourly A between 0800 and 1700 h.

observed A by Valle et al. (1985) at elevated $[CO_2]$ are very high, and two different simulation models were not able to reproduce these high leaf photosynthetic rates. Our underprediction by 20% is in the same range as the 14 to 24% underpredictions that Grant reported. It is possible that CO_2 leakage from the leaf chamber system associated with steeper gradient from elevated $[CO_2]$ to ambient could have contributed to greater observed A.

Simulated and observed A agreed closely at ambient $[CO_2]$ (Table 2). The RMSE was 15% of the observed mean A, indicating that the model captured most of the variation in observed A. The proportion of unsystematic mean squared error (MSE_u) (equivalent to $RMSE_u{}^2$) to MSE (equivalent to $RMSE^2$) was high (87%), and the proportion of systematic mean squared error (MSE_s) (equivalent to $RMSE_s{}^2$) to MSE was only 13%. Low values of MSE, values of MSE_u approaching MSE, and values of MSE_s approaching zero are measures of a "good model." The D index was 0.97, reflecting the degree to which the observed A was accurately estimated by the model at ambient $[CO_2]$. Unlike simulation of A in ambient $[CO_2]$, RMSE was 25% of the observed mean A at elevated $[CO_2]$. The proportion MSE_s to MSE was high (84%), indicating that the model did not predict well at high $[CO_2]$, although the D index was 0.93.

The model predicted that doubled $[CO_2]$ from 330 to 660 μmol mol⁻¹ increased simulated A (at PPF >1100 μmol m⁻² s⁻¹) by 52%, similar to values of most published studies. The simulated doubled $[CO_2]$ effect on A for soybean was similar to the 48% increase reported by Vu et al. (1997), the 39% increase reported by Ainsworth et al. (2002), and the 45% increase reported by Booker et al. (2005). In contrast, Valle et al. (1985) reported an increase of 93% due to doubling of $[CO_2]$. The simulated quantum efficiency by the CROPGRO model at 330 and 660 μmol CO_2 mol⁻¹ was 0.050 and 0.064 μmol CO_2 mol⁻¹ quanta, respectively, which compares well with values reported by Ehleringer and Björkman (1977).

Response of Leaf Photosynthesis to Intercellular Carbon Dioxide Concentration

The primary source of biochemical limitation to A depends generally on the C_i. It is therefore important to evaluate CROPGRO model predictions of A/C_i response. We compared simulated A/C_i curves to observed A/C_i data from Valle et al. (1985), Harley et al. (1985), Sims et al. (1998), and Griffin and Luo (1999). Observed
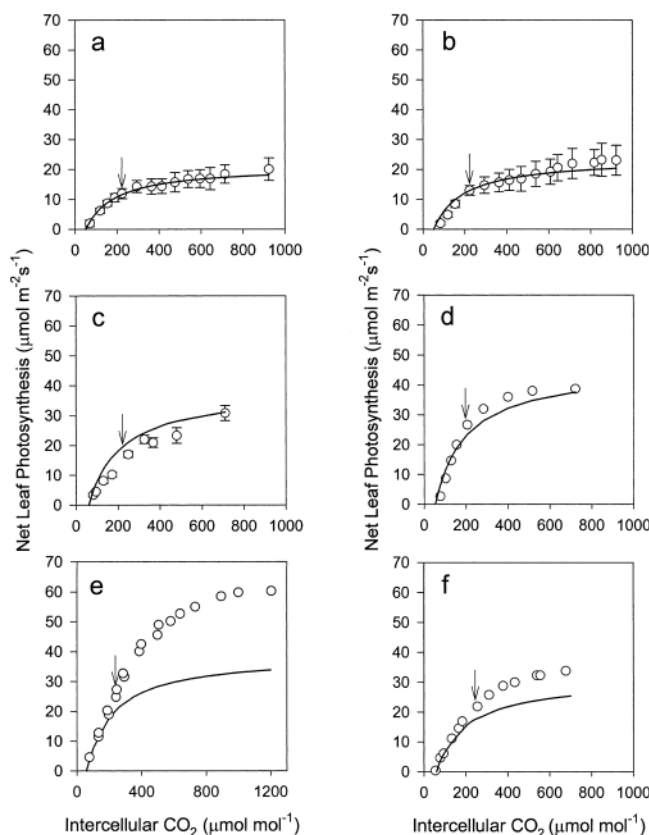

Fig. 2. Simulated net leaf photosynthesis (A) of soybean as a function of intercellular $[CO_2]$ (C_i). Symbols are for measured data (mean ± SD, adapted from references), and curves are for simulations using default CROPGRO photosynthetic equations. Panels (a) and (b) are from Griffin and Luo (1999) for plants grown in 350 and 700 μmol CO_2 mol⁻¹, respectively; panel (c) is from Valle et al. (1985); panel (d) is from Sims et al. (1998); panel (e) and (f) are from the high- and low-light experiments, respectively, of Harley et al. (1985). Arrows indicate the intercellular $[CO_2]$ equivalent to ambient $[CO_2]$.

and simulated A responded asymptotically to increases in C_i in all data sets with an initial steep slope at subambient $[C_i]$, where A is generally limited by Rubisco activity (Fig. 2). Simulated and observed A/C_i curves exhibited a gradual saturation as C_i increased above ambient $[C_i]$ and approached the RuBP-regeneration limited part of the A/C_i response curve. This response of A to C_i is expected because increased $[CO_2]$ provides more substrate for carboxylation and overcomes the competitive inhibition of Rubisco enzyme by oxygen. The simulated A/C_i curves showed similar responses as reported by Griffin and Luo (1999), Valle et al. (1985),
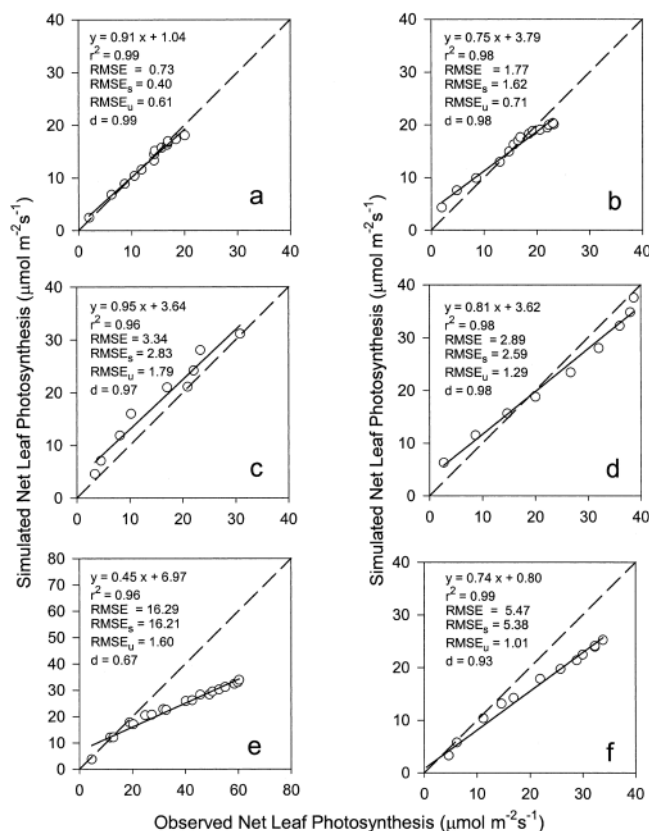
Fig. 3. Comparison of observed (data adapted from references) and simulated net leaf photosynthesis using default CROPGRO photosynthetic equations. (a) Griffin and Luo (1999) for plants grown in 350 μmol CO_2 mol^{-1}; (b) Griffin and Luo (1999) for plants grown in 700 μmol CO_2 mol^{-1}; (c) Valle et al. (1985); (d) Sims et al. (1998); (e) Harley et al. (1985) (at high light, PPF > 2000 μmol photon m^{-2} s^{-1}); and (f) Harley et al. (1985) (at low light, PPF $\approx$ 800 μmol m^{-2} s^{-1}). Solid lines show linear regression, and dashed lines show the 1:1 line.

and Sims et al. (1998) (Fig. 2a–d). In contrast, the model underpredicted A at all C_i levels above ambient $[CO_2]$ in the data sets from Harley et al. (1985) (Fig. 2e–f). In their high light level experiment, the observed A at 1200 μmol mol^{-1} C_i was 60 μmol m^{-2} s^{-1}, whereas the model predicted 34 μmol m^{-2} s^{-1}. One reason for this anomaly could be that very high light levels were used during A measurement (PPF > 2000 μmol m^{-2} s^{-1}), whereas the plants were grown at low light levels (PPF $\approx$ 800 μmol m^{-2} s^{-1} (Table 1). In a low light experiment by Harley et al. (1985), the observed A was 32.3 μmol m^{-2} s^{-1} (at 560 μmol mol^{-1} C_i and PPF $\approx$ 800 μmol photon m^{-2} s^{-1}), compared with 50.6 μmol m^{-2} s^{-1} (at 580 μmol mol^{-1} C_i and PPF > 2000 μmol photon m^{-2} s^{-1}) measured by Harley et al. (1985) in the high light level experiment. The simulated A was 24.6 μmol m^{-2} s^{-1} at 600 μmol mol^{-1} C_i and PPF of 800 μmol photon m^{-2} s^{-1}.

The observed and simulated A clustered along the 1:1 line in Valle et al. (1985), Sims et al. (1998), and Griffin and Luo (1999) data sets (Fig. 3a–d). The size of RMSE as the percentage of the observed mean A ranged from 5 to 21%. The D indices were all high, explaining most of the variations in the observed A. In contrast, the model underpredicted A in the high light

experiment of the Harley et al. (1985) data set (D = 0.67), where the light environment for plant growth and A measurement were greatly different. In this data set, A values fell below 1:1 when observed A was above 20 μmol m^{-2} s^{-1} (Fig. 3e). The size of RMSE compared with the observed mean A was 44%, and the D index was low, indicating that the model did not explain most of the variations in observed A. However, in a low light experiment (Harley et al., 1985) where the light environment for plant growth and A measurement were the same, the simulated A values were closer to the 1:1 line (Fig. 3f), the ratio of RMSE to observed mean A was 27%, and the D index was high. Considering the high D indices and low variance (RMSE was 5–27% of mean) for five of the six data sets used for model evaluation, our analysis indicated that the CROPGRO default photosynthetic equations reasonably simulate the A/C_i curves. The underprediction of A in one experiment by Harley et al. (1985) was an exception, and CO_2 leakage could have caused higher A, especially under high light (PPF > 2000 μmol m^{-2} s^{-1}).

The current leaf photosynthesis equations in the CROPGRO model accurately simulated the response of A to $[CO_2]$ because they reproduced the A/C_i curves and the average doubled $[CO_2]$ effect on A that have been reported in the literature. Doubling $[CO_2]$ from ambient increased simulated A_{sat} by 41, 38, and 36% (mean 38%) in comparison to the observed A_{sat} increase of 61, 35, and 31% (mean 41%) in the Harley et al. (1985), Sims et al. (1998), and Griffin and Luo (1999) data sets, respectively. This simulated response of A to the doubling of $[CO_2]$ compares well with the 39% average increase reported with doubling of $[CO_2]$ summarized from 78 studies in the meta-analysis of soybean by Ainsworth et al. (2002), with the 49% increase reported by Vu et al. (1997) when $[CO_2]$ was increased from 350 to 700 μmol CO_2 mol^{-1}, with the 45% increase reported by Booker et al. (2005), and with the 52% increase due to $[CO_2]$ doubling reported for various crops (Cure and Acock, 1986).

Comparison of CROPGRO's Default Photosynthesis Equations to Farquhar Photosynthesis Equations

The CROPGRO default photosynthesis equations and the Farquhar photosynthesis equations predicted A/C_i response reasonably well in Griffin and Luo data sets (Fig. 4a, b). CROPGRO predicted A/C_i response well for the Sims et al. (1998) data set, but the Farquhar equations did not, and the Farquhar equations underpredicted A/C_i response at all levels of C_i (Fig. 4c). Sims et al. (1998) derived the $V_{c,max}$ using kinetic parameters K_c and K_o. The derivation of $V_{c,max}$ value strongly depends on the use of correct K_c and K_o values. The parameter J_{max} was linearly related to $V_{c,max}$ in 109 crop species (Wullschleger, 1993) and in soybean (Griffin and Luo, 1999). Sims et al. (1998) reported 83.6 and 184.8 μmol m^{-2} s^{-1} for $V_{c,max}$ and J_{max}, respectively. However, based on the linear relationship between $V_{c,max}$ and J_{max} developed by Griffin and Luo (1999) for soybean, the revised
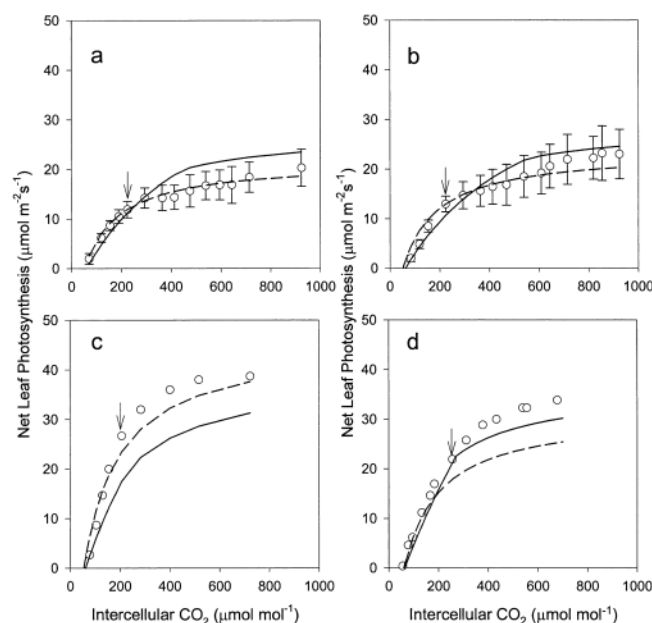
Fig. 4. Comparison of observed (symbols) (data adapted from references) and simulated A using the default CROPGRO photosynthetic equations (dashed lines) or the full Farquhar photosynthetic equations (solid lines). (a) Griffin and Luo (1999) for plants grown in 350, (b) Griffin and Luo (1999) for plants grown in 700 μmol CO_2 mol^{-1}, (c) Sims et al. (1998), and (d) Harley et al. (1985). Arrows indicate the intercellular [CO_2] equivalent to ambient [CO_2] treatments.

component of RMSE for predictions of A by both models. The D indices ranged from 0.90 to 0.99 for all the data sets used in model evaluation, indicating that the CROPGRO and Farquhar equations were equally efficient in predicting A over a range of C_i.

Response of Canopy Photosynthesis to Photosynthetic Photon Flux and Carbon Dioxide Concentration

CROPGRO responses of A are integrated over sunlit and shaded leaf classes. The model simulates vertical gradients in SLW and leaf N concentration with LAI depth. The SLW and leaf N concentration are highest for upper leaves (which maximizes upper leaf response to higher irradiance) and decline progressively toward the bottom of the canopy to affect A_{max} with LAI depth (Boote and Pickering, 1994). Because canopy photosynthesis plays a vital role in determining the consequences of [CO_2] on primary productivity, it is important to evaluate the capabilities of the CROPGRO model to predict the response of A_{can} to PPF at different [CO_2].

Simulated and observed A_{can} increased with increasing PPF at all [CO_2] (Fig. 5). Observed A_{can} light saturated at 800 μmol m^{-2} s^{-1} at the two lowest [CO_2], but simulated A_{can} continued to increase at higher light for the higher [CO_2] treatments (Fig. 5). Observed A_{can} was not light saturated even at 1300 μmol m^{-2} s^{-1} for [CO_2] above 280 μmol mol^{-1}. With the assumption of PPF

Table 3. Mean ($\pm$ SD) of observed and simulated net leaf photosynthesis using the full Farquhar and von Caemmerer (1982) equations or the default CROPGRO equations. Shown also are Willmott's index of agreement and root mean square error and its systematic and unsystematic components.

Data source	Observed A† (mean $\pm$ SD)	Simulated A (mean $\pm$ SD)		D index		RMSE		RMSE$_s$		RMSE$_U$	
		(1)‡	(2)§	(1)	(2)	(1)	(2)	(1)	(2)	(1)	(2)
	——— μmol m^{-2} s^{-1} ———							——— μmol m^{-2} s^{-1} ———			
Harley et al. (1985)	19.9 $\pm$ 11.69	17.3 $\pm$ 11.2	15.4 $\pm$ 8.65	0.99	0.93	2.73	5.47	2.63	5.38	0.73	1.01
Sims et al. (1998)	24.2 $\pm$ 13.32	17.3 $\pm$ 10.4	23.2 $\pm$ 10.87	0.90	0.98	7.53	2.89	7.39	2.59	1.47	1.29
Griffin and Luo (1999)¶	13.3 $\pm$ 5.01	15.4 $\pm$ 7.39	13.6 $\pm$ 4.73	0.93	0.99	3.29	0.73	2.89	0.40	1.57	0.61
Griffin and Luo (1999)#	16.1 $\pm$ 6.55	17.1 $\pm$ 7.78	15.8 $\pm$ 4.95	0.98	0.98	2.03	1.77	1.50	1.62	1.37	0.71

† A, net leaf photosynthesis; D, Willmott's index of agreement; RMSE, root mean square error; RMSEs, systematic component of the root mean square error; RMSE$_u$, unsystematic component of the root mean square error.
‡ (1) Farquhar and von Caemmerer (1982) photosynthetic equations.
§ (2) CROPGRO photosynthetic equations.
¶ Plants grown at [CO_2] 350 μmol mol^{-1}.
# Plants grown at [CO_2] 700 μmol mol^{-1}.

value for J_{max} for Sims et al. data should be 220.0 μmol m^{-2} s^{-1} rather than 184.8 μmol m^{-2} s^{-1}. One reason for the lower predictions of A at all levels of C_i in Sims et al. (1998) data by the Farquhar equations could be the use of lower J_{max} values. The predictions of A for Harley et al. (1985) data by both models were reasonably good at C_i levels below 200 μmol mol^{-1}, but both underestimated A in the RuBP-limited portion of the A/C_i response curve (Fig. 4d).

The Farquhar equations were not superior to CROPGRO's equations for simulating A. Over all the data sets, the mean RMSE for predictions of A by the CROPGRO equations was 2.72, compared with 3.89 for predictions of A by the Farquhar equations (Table 3), indicating that CROPGRO's equations simulated A more closely than did the Farquhar equations. The RMSE$_s$ was the major

transmission of 0.88, the simulations underpredicted A_{can} at [CO_2] above 280 μmol mol^{-1} when the PPF was above 400 μmol m^{-2} s^{-1}. The recorded PPF shown on the x axis of Fig. 5 was measured outside and above the chambers; however, the initial simulations were done assuming 88% transmission of PPF through chamber walls (transmission measured for this chamber covering material). However, simulations by Kim et al. (2004) for comparable sunlit chambers showed that on a clear day at a height of 0.5 m from soil surface the crop growing area inside sunlit chambers received 108% of ambient PPF because of reflected light from back panels and side panels of the sunlit chambers. To the extent that inside-chamber PPF is higher than what we assumed [from Kim et al. (2004) analyses], the model would be expected to underestimate A_{can} compared with
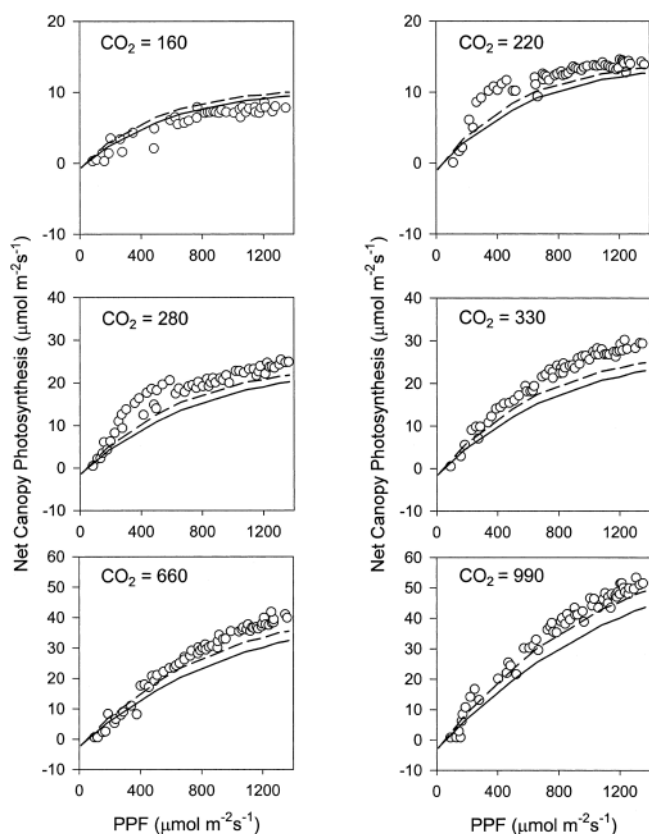
Fig. 5. Simulated soybean net A_{can} as a function of PPF at six [CO_2]. Symbols are from observed data at 5-min intervals (adapted from Campbell et al., 1990), and curves are from simulation by the CROPGRO model using hourly PPF between 0600 and 1700 h, with assumption of PPF transmission of 0.88 (solid lines) or PPF transmission of 1.08 (dashed lines). The PPF on the x axis is external to and above the chamber walls.

Fig. 6. Comparison of observed (adapted from Campbell et al., 1990) and simulated net A_{can} by the CROPGRO model at six [CO_2], assuming PPF transmission of 1.08. Linear regression using hourly observed and simulated A_{can} values from 0700 to 1700 h (solid lines) and 1:1 line (dashed lines).

the observed A_{can}, especially for larger canopies. To test the influence of possible increase in the radiation environment inside the sunlit chambers, Fig. 5 shows a comparison of simulated A_{can} using PPF transmission factor of 0.88 or 1.08. With an assumption of 1.08 transmission, the simulated A_{can} for various [CO_2] was much closer to the observed A_{can} at all but the lowest [CO_2] (Fig. 5). Furthermore, some of the remaining underprediction of A_{can} at higher [CO_2] could be attributed to the greater fraction diffuse PPF in the chambers that the model did not predict (with higher PPF, the model predicts less diffuse PPF). The model computes fraction diffuse PPF based on actual radiation compared with the solar constant.

Moreover, using a multilayer canopy light interception model, simulations of *Cecropia peltata* L. (a fast-growing tropical tree species) by Allen et al. (1974) indicated that A_{can} increased slightly with increasing fraction diffuse PPF (up to nearly 0.60 diffuse PPF) even as total global PPF was decreasing across this range. This impact of fraction diffuse PPF on A_{can} is further supported by the review by Sinclair and Muchow (1999), wherein radiation use efficiency (crop biomass accumulation per unit solar radiation intercepted) was increased as fraction diffuse PPF increased.
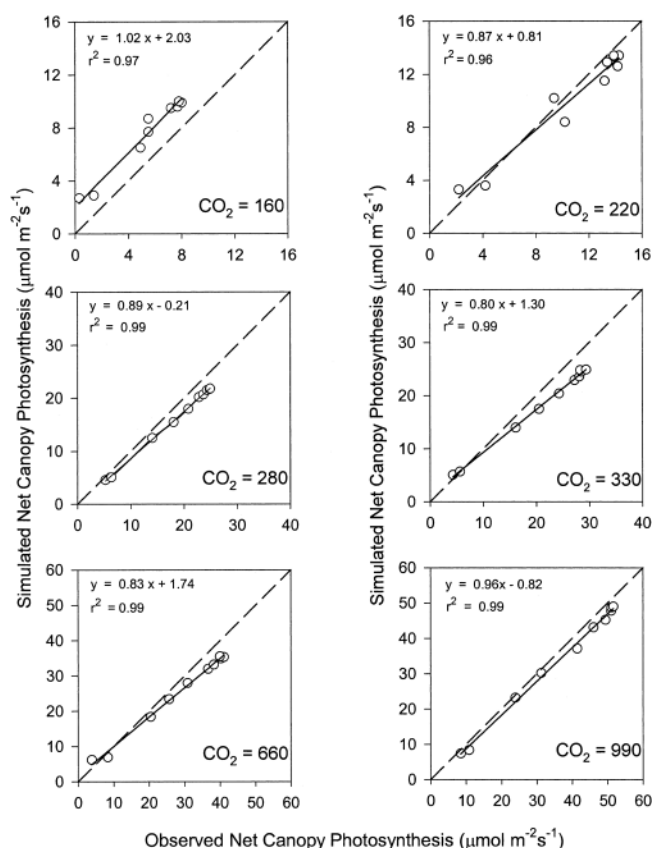
With the 1.08 transmission assumption, the simulated

and observed A_{can} clustered close but somewhat below the 1:1 line in all [CO_2] except at 160 and 220 µmol mol^{-1} (Fig. 6). The D index values ranged from 0.96 to 0.99 in all but the lowest [CO_2], reflecting the degree to which the simulated A_{can} compares with the observed. The RMSE expressed as a percentage of observed mean A_{can} ranged from 8 to 16% in all but the lowest [CO_2], giving a good overall measure of model performance and complementing the D index. A full statistical comparison in Table 4 shows the general improvement in the model predictions (lower RMSE, especially lower $RMSE_s$, and higher D index) when PPF transmission of 1.08 is assumed compared with 0.88. The decomposition of RMSE indicated a generally higher systematic error ($RMSE_s$) than random error ($RMSE_U$), especially for the 0.88 transmission assumption. The substantial decrease in $RMSE_S$ associated with switch from 0.88 to 1.08 transmission factor is the type of error that could be associated with failure to account for the reflected radiation from the side and back walls of the chambers. Even with the 1.08 transmission assumption, the model still slightly underpredicts, as evidenced by the slopes being less than unity, but increasing the fraction diffuse PPF would also improve this situation. Considering the high D index and low ratio of RMSE compared with the observed mean A_{can} (ratios of 8–16%), our analysis indicates acceptable agreement between the observed

Table 4. Mean $\pm$ SD of 11 hourly observed (Campbell et al., 1990) and simulated net canopy photosynthesis from CROPGRO model for six CO_2 concentrations. Simulations of net canopy photosynthesis were done with transmission factors of 0.88 and 1.08 of photosynthetic photon flux external to and above the chambers. Also shown are the root mean square error, its systematic and unsystematic components, and Willmott's index of agreement for both simulations.

[CO₂]	A_{can}† (mean $\pm$ SD)‡			Statistics for simulations with PPF transmission factor 0.88				Statistics for simulations with PPF transmission factor 1.08			
		Simulated									
	Observed	PPF*0.88	PPF*1.08	RMSE	RMSE$_s$	RMSE$_u$	D	RMSE	RMSE$_s$	RMSE$_u$	D
μmol mol⁻¹		μmol m⁻² s⁻¹							μmol m⁻² s⁻¹		
160	5.6 $\pm$ 2.76	7.1 $\pm$ 2.83	7.7 $\pm$ 2.85	1.59	1.53	0.45	0.92	2.18	2.12	0.45	0.86
220	10.9 $\pm$ 4.42	9.5 $\pm$ 4.42	10.3 $\pm$ 3.91	1.73	1.55	0.77	0.95	1.12	0.84	0.74	0.98
280	18.5 $\pm$ 7.53	14.6 $\pm$ 6.39	16.1 $\pm$ 6.67	4.02	4.01	0.28	0.92	2.47	2.46	0.20	0.97
330	21.2 $\pm$ 9.54	16.5 $\pm$ 7.31	18.3 $\pm$ 7.67	5.20	5.17	0.51	0.90	3.42	3.40	0.37	0.96
660	28.5 $\pm$ 13.66	22.6 $\pm$ 10.63	25.4 $\pm$ 11.38	6.56	6.52	0.75	0.92	3.86	3.78	0.79	0.97
990	36.5 $\pm$ 16.87	29.7 $\pm$ 14.69	34.0 $\pm$ 16.14	7.13	7.08	0.86	0.95	2.76	2.59	0.95	0.99

† A_{can}, net canopy photosynthesis; [CO₂], carbon dioxide concentration; D, Willmott's index of agreement; RMSE, root mean square error; RMSE$_s$, systematic component of the root mean square error; RMSE$_u$, unsystematic component of the root mean square error.
‡ Mean $\pm$ SD of 11 hourly observed (O_i) and simulated (P_i) net canopy photosynthesis.

and simulated A_{can} at sub- and supraoptimal [CO₂] by the CROPGRO model.

Doubling of [CO₂] from the ambient (330 μmol CO_2 mol⁻¹) increased simulated A_{can} (at 1350 μmol m⁻² s⁻¹ PPF) by 42% and observed A_{can} by 36%. The effect of doubling [CO₂] on simulated A_{can} in this study is similar to the 59% increase (range of 40–87%, using 95% confidence interval) summarized in the soybean meta-analysis (Ainsworth et al., 2002).

CONCLUSIONS

We used leaf and canopy photosynthesis data obtained from environmentally controlled [CO₂] enrichment experiments on soybean to test the ability of the unmodified CROPGRO soybean model to accurately simulate responses of A and A_{can} to PPF and the response of A to C_i. Simulated A closely matched observed A (Valle et al., 1985) at all PPF levels at ambient [CO₂], but the model underpredicted A on high PPF at elevated [CO₂]. Two other modeling studies have reported similar underprediction of A at elevated [CO₂] for this particular data set.

Simulated A/C_i curves were similar to the observed curves in most cases. Comparison of observed and simulated A, A_{can}, and A/C_i curves indicated a high D, varying from 0.93 to 0.99, and deviation-based RMSE were small compared with the respective observed mean A and A_{can}. Simulated and observed A_{can} light saturated at 800 μmol m⁻² s⁻¹ PPF below 280 μmol mol⁻¹ [CO₂] but did not light saturate even at 1300 μmol m⁻² s⁻¹ PPF above 280 μmol mol⁻¹ [CO₂]. The simulation of effects of doubling [CO₂] on A and A_{can} were comparable to increases summarized in the soybean meta-analysis (Ainsworth et al., 2002). Even though the CROPGRO model uses a simplification based on the RUBP-limiting equations of Farquhar and von Caemmerer (1982), our comparison using common data sets indicated that the CROPGRO default photosynthesis equations and the Farquhar photosynthesis equations were equally effective in simulating A over a range of C_i. This model evaluation study indicated that the CROPGRO model with default photosynthesis equations adequately simulated the response of A and A_{can} to PPF and the response of A to

[C_i]. Simulated doubled [CO₂] effects on A and A_{can} matched closely to the values reported in the literature.

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