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Decomposition analysis on soybean productivity increase under elevated CO₂ using 3-D canopy model reveals synergistic effects of CO₂ and light in photosynthesis

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• Background and Aims Understanding how climate change influences crop productivity helps in identifying new options to increase crop productivity. Soybean is the most important dicotyledonous seed crop in terms of planting area. Although the impacts of elevated atmospheric [CO₂] on soybean physiology, growth and biomass accumulation have been studied extensively, the contribution of different factors to changes in season-long whole crop photosynthetic CO₂ uptake [gross primary productivity (GPP)] under elevated [CO₂] have not been fully quantified.

• Methods A 3-D canopy model combining canopy 3-D architecture, ray tracing and leaf photosynthesis was built to: (1) study the impacts of elevated [CO₂] on soybean GPP across a whole growing season; (2) dissect the contribution of different factors to changes in GPP; and (3) determine the extent, if any, of synergism between [CO₂] and light on changes in GPP. The model was parameterized from measurements of leaf physiology and canopy architectural parameters at the soybean Free Air CO₂ Enrichment (SoyFACE) facility in Champaign, Illinois.

• Key Results Using this model, we showed that both a CO₂ fertilization effect and changes in canopy architecture contributed to the large increase in GPP while acclimation in photosynthetic physiological parameters to elevated [CO₂] and altered leaf temperature played only a minor role in the changes in GPP. Furthermore, at early developmental stages, elevated [CO₂] increased leaf area index which led to increased canopy light absorption and canopy photosynthesis. At later developmental stages, on days with high ambient light levels, the proportion of leaves in a canopy limited by Rubisco carboxylation increased from 12.2 % to 35.6 %, which led to a greater enhancement of elevated [CO₂] to GPP.

• Conclusions This study develops a new method to dissect the contribution of different factors to responses of crops under climate change. We showed that there is a synergistic effect of CO₂ and light on crop growth under elevated CO₂ conditions.

Key words: Canopy architecture, photosynthesis, atmospheric change, climate change, food security, growth, leaf temperature, canopy absorbance, leaf area index, light extinction coefficient, soybean, SoyFACE.

INTRODUCTION

Soybean is the most important dicotyledonous seed crop in terms of area planted and mass produced at the global scale. It is also the largest single source of vegetable protein for food and feed in the world. Understanding the response of soybean growth and productivity to global atmospheric change will be critical to an accurate projection of future soybean production and global food security (Parry et al., 2004; Long et al., 2006). The impacts of elevated [CO₂] on soybean physiology, growth and development have been extensively documented (Kimball, 1983; Ainsworth et al., 2002; Bernacchi et al., 2005, 2006, 2007; Morgan et al., 2005). Soybean grown under free air [CO₂] enrichment shows a 37 % increase of biomass dry weight and 24 % increase in yield with a [CO₂] increase to about 700 ppm (Ainsworth et al., 2002). When [CO₂] is increased to about 550 ppm, above-ground biomass increases by 17–18 % and yield increases by 15 % (Morgan et al., 2005). The yield increase is significant, but less than the expected increase under elevated [CO₂] (Long et al., 2006). Similar observations of lower than expected increase in crop yields under elevated [CO₂] have been made in other species as well (Long et al., 2004).

To a first approximation, the yield of a crop under optimal growth conditions is the product of the solar radiation receipt for the growing season and the efficiencies with which the crop intercepts that radiation (εᵣ), converts it into biomass (εₑ) and partitions the biomass into the harvested organ (εₑ), i.e. seed in the case of soybean (Monteith, 1972). Under elevated [CO₂], the partitioning efficiency (also known as harvest index) of soybean is only slightly reduced, compared to under ambient [CO₂]. Measured harvest index is about 0.55 and 0.53 for
In this study, we use a 3-D canopy photosynthesis model to dissect the contribution of different environmental, architectural and physiological parameters to the changes in GPP under elevated CO₂. Using the model, we further show that there is a synergistic effect between [CO₂] and light for soybean grown under elevated CO₂.

**MATERIALS AND METHODS**

**SoyFACE facility**

The data used for model parameterization in this study were collected from the SoyFACE facility (www.soyface.uiuc.edu), which employs a free air concentration enrichment (FACE) technology. SoyFACE is a 32-ha facility at the University of Illinois at Urbana-Champaign (40°03′21.3″N, 88°12′3.4″W, 230 m elevation). The soil at SoyFACE is a Drummer-Flanagan series (fine-silty, mixed, mesic Typic Endoaquoll; Morgan et al., 2005), typically very deep and formed from loess and silt parent material deposited on the till and outwash plains. The average ground surface slope is <1 % at this site, with tile drains at a depth of 1–2 m below the ground surface. This rain-fed field site has been following a continuous crop rotation practice typical for the US Midwestern corn belt of soybean and maize. Extended descriptions of site, including micrometeorology and climate, have been previously described (Leakey et al., 2004; Rogers et al., 2004).

SoyFACE elevated [CO₂] treatments consist of four blocks each with two octagonal plots of 20 m diameter within the 16 ha planted with soybean. Each block contains one control plot at an ambient [CO₂] of 370 ppm and one fumigated plot to a target [CO₂] of 550 ppm, using the FACE technology of Miglietta et al. (2001). Fumigation was performed between sunrise and sunset and began 3 d after planting and operated over the remainder of the growing season until crop harvest.

**Leaf photosynthetic parameters**

\[ V_{c\text{max}} \text{ and } J_{\text{max}} \text{ of canopy top leaves for ambient and elevated [CO₂] were taken from Morgan et al. (2005). An exponential distribution model was used to predict } V_{c\text{max}} \text{ and } J_{\text{max}} \text{ for leaves at different depth (z) of the canopy (eqn 1) following previous observations of } V_{c\text{max}}, J_{\text{max}} \text{ and leaf nitrogen content in different layers of the canopy (Morgan et al., 2004; Srinivasan et al., 2016). The relationship between } V_{c\text{max}} \text{ and cumulative leaf area index (cLAI) from the top of the canopy was based on the vertical distribution of leaf nitrogen content in the canopy. } V_{c\text{max,top}} \text{ is the } V_{c\text{max}} \text{ of leaves in the top layer of a canopy.} \]

\[ V_{c\text{max}}(z) = V_{c\text{max,top}} \cdot \exp \left(-0.2 \cdot c\text{LAI}(z) \right) \]  

(1)

**Meteorological parameters**

Air temperature (°C), relative humidity, photosynthetic photon flux density (PPFD) and diffuse PPFD were recorded with 10-min intervals at the weather station located at SoyFACE.
**Calculation of GPP**

The overall workflow used to calculate GPP was as follows: (1) development of a 3-D soybean canopy photosynthesis model; (2) simulation of the light environments inside a canopy; (3) calculation of the photosynthetic rate of each leaf; and (4) calculation of the canopy photosynthetic rate by integrating the total photosynthetic rate for all leaves in a canopy. These steps are described in detail in the following sections.

**3-D soybean canopy model**

A 3-D soybean canopy model was developed based on the 3-D canopy modelling algorithm of Song et al. (2013) (the MATLAB-based program, mCanopy-soybean, is available from the authors upon request).

The different measurements required for the 3-D canopy model development are summarized in Supplementary Data Tables S1–S8. Leaf lengths, leaf widths, petiole lengths and angles for the left, middle and right trifoliate leaves (Tables S1–S3) were obtained using digital photography and image processing. An in-situ non-destructive leaf photo scanner was used to obtain a picture of the soybean trifoliate leaves at all nodes for five plants per plot. The scanner holds a leaf between two flat sheets, with the top sheet being transparent, to obtain a photo of the leaf. A standard length was placed within the frame of the picture for reference. The camera was mounted normal to the leaf plane and the leaf image was recorded using a digital camera. Leaf widths, lengths and the angles were digitally processed using the java-based image processing and analysis software ImageJ (1.48j 11 December 2013, https://imagej.nih.gov/ij/).

The internode lengths and petiole lengths (Supplementary Data Table S4) for each node in the main stem and the branches were measured for the same five plants in each plot using a ruler. Petiole angle, branch angle and leaf angle were measured using a protractor (iGaging digital protractor, http://www.igaging.com/) at midday. These measurements were made for the same five plants in each plot.

Measurements of leaf senescence were made on the same five plants in each plot, recorded twice a week for each node. Leaves that turned pale yellow to brown were considered non-photosynthetic and senesced. Note that there was a finite duration of time between post-yellowing of leaves and complete litterfall (a few days to a week). In our 3-D model, we assume all leaves that turned yellow have senesced. During the growing season, ten plants from each plot were identified to measure development, and the presence of branches and their node lengths were measured. Using these data, a branching probability was computed (Supplementary Data Tables S5–S7).

A soybean architecture model (features in Fig. 1A–C) was developed based on these measured architecture data. The description of nodes and branches is given in Table 1. In the main stem, the base node before the first node is the VU node, which is the node growing unifoliate leaves (Fig. 1A), and the first trifoliate leaf is on the first node V1. The second trifoliate leaf grows on the second node V2 and so on. The first branch (Br1) grows from the V1 node and the second branch (Br2) from the V2 node and so on. Internode length is the distance between two nodes (e.g. V3 internode length was the length between nodes V3 and V2). Branch angle is the angle between the main stem and branch (Fig. 1B), petiole angle 1 is the angle between the main stem (or branch) and the common petiole of a trifoliate leaf (Fig. 1C), and petiole angle 2 (Fig. 1B) is the angle between a common petiole and the petiole of the mid-leaf of the trifoliate leaf. Mid-leaf angle is the angle between the petioles of the mid-leaf and the main vein of the mid-leaf (Fig. 1b). Leaf length and leaf width are the maximal length and width of a leaf. Leaf angle L, leaf angle R and leaf angle M (Fig. 1C) are the angles between the common petiole of a trifoliate leaf and the main veins of left, right and middle leaves when these leaves are laid on a horizontal plane.

**3-D soybean canopy models applied to different days in the growing season**

Row spacing was 38 cm and the planting distance was 5 cm under both ambient and elevated CO2 conditions. The integrated model was run for the year 2002 between days 168 (V1) and 267 (V16) every 3 d (Fig. 1D, E).

To simulate canopy photosynthesis throughout a growing season (Fig. 1), canopy architectural parameters (i.e. leaf length, leaf width, leaf angle, internode length, etc.) were measured at different stages of plant growth (Supplementary Data Tables S1–S4). To model the variation of node number among different plants, we used a randomization algorithm to determine the node number (Vx) for each main stem and branch as follows.

First, the maximal node number (Vx_max) for the main stem and branches for different days of the year (DOY) were determined based on previous measurements (Castro et al., 2009). Second, the probability p(n) (probability for node number = n) of the main stem or branches on different days were calculated based on measurement data (Supplementary Data Table S8). A random value between 0 and 1 (uniform distribution) was then generated and if i > sum(p(n<=n)) and i < sum(p(n>N)) (probability for node number = n) is used for Vx_r, which is the randomized node number. Lastly, if Vx_r is less than Vx_max, Vx_r is used as the node number, and if Vx_r is larger than Vx_max, Vx_max is used as the node number (Tables S5–S7). Pseudocode for the above process is given in the Supplementary data Methods.

Senesced leaves were excluded from the model. The number of senesced leaves was counted during the growing season and the number of senesced leaves every 3 d was based on measurement data (Supplementary Data Table S8). The total number of senesced leaves (Vx) on a DOY is the sum of the senesced leaf number from the start day (168 DOY) to the current day. If Ns is not an integer, a randomization algorithm is used to determine the total senesced leaf number. For example, if Ns = 2.3, then leaf number being 2 is used with a probability of 0.7 and leaf number being 3 is used with a probability of 0.3. In the model, newly formed leaves were smaller than mature leaves. The sizes of the top three newest formed leaves (from top to bottom) were assumed to be 25 %, 50 % and 75 % of their mature sizes.

**Ray tracing algorithm**

The light environment in the soybean canopy was simulated using a ray tracing algorithm, fastTracer (Song et al., 2013).
The program for fastTracer is available upon request from the corresponding author. Measured ambient direct and diffuse photosynthetic photon flux density (PPFD) data were used as input to fastTracer. The ray tracing algorithm simulates the direct PPFD, diffuse PPFD and leaf scattering PPFD absorbed by every leaf. The simulations were conducted 15 times a day, from 0500 to 1900 h with intervals of 1 h. Using ray tracing, the calculation of PPFD distribution in the canopy was accurate for evaluating the impacts of small differences in canopy architecture, such as leaf size and leaf number and the PPFD distribution under different weather conditions, both of which were important for this study.

**Leaf photosynthesis calculation**

Leaf photosynthetic CO₂ uptake rate was calculated with the steady-state biochemical model of C₃ leaf photosynthesis (Farquhar et al., 1980).

Leaf photosynthesis rate at any given CO₂, light, O₂ and temperature conditions was calculated from eqn (2):

\[
P = \left(1 - \frac{C_i^*}{C_i}ight) \cdot \min\{W_c, W_f\}
\]

where: \(C_i^*\) is the CO₂ compensation point in the absence of dark respiration, \(C_i\) is the leaf intercellular CO₂ concentration, \(W_c\) is
the Rubisco-limited rate of carboxylation and \( W_c \) is the RuBP regeneration-limited rate of carboxylation, which were calculated from eqns (3) and (4):

\[
W_c = \frac{V_{c\max} \cdot C_i}{C_i + K_c \cdot [1 + \frac{C_s}{C_i}]} \tag{3}
\]

\[
W_j = \frac{J \cdot C_i}{4.5 \cdot C_i + 10.5 \cdot \Gamma s} \tag{4}
\]

where \( K_c \) is the Michaelis constant for CO\(_2\) (404.9 \( \mu \)mol mol\(^{-1}\)), \( K_s \) is the Michaelis constant for O\(_2\) (278.4 \( \mu \)mol mol\(^{-1}\)) and \( J \) is the potential photosynthetic electron transport rate. The parameters describing impacts of temperature on Rubisco kinetics follow Bernacchi et al. (2001). Leaf temperature was assumed to be equal to air temperature \( T \) for the ambient condition and leaf temperature was assumed to be 1.5 °C higher under elevated CO\(_2\) than under ambient conditions based on the data from Long et al. (2006).

The potential electron transport rate, \( J \), was calculated as:

\[
J = \frac{I_2 + J_{\max} - \sqrt{(I_2 + J_{\max})^2 - 4 \cdot \Theta_{PSII} \cdot I_2 \cdot J_{\max}}}{2 \cdot \Theta_{PSII}} \tag{5}
\]

where \( \Theta_{PSII} \) (0.864 was used) is the convexity of the non-rectangular curve, \( I_2 \) is the PPFD absorbed by photosystem II (PSII), and \( J_{\max} \) is the maximal electron transport rate (Chen, Zhu & Long, 2008). \( I_2 \) was calculated from:

\[
I_2 = I_{sun} \cdot \alpha_I \cdot \Phi_{PSII,\max} \cdot \beta \tag{6}
\]

where \( I_{sun} \) is the PPFD incident upon a facet in a leaf simulated by the ray tracing algorithm described by Song et al. (2013), \( \alpha_I \) is leaf absorbance (0.85 was used), \( \Phi_{PSII,\max} \) is the maximal quantum yield of PSII (0.85 was used) and \( \beta (0.5 \text{ was used}) \) is the maximal fraction of quanta that reaches PSII (Chen et al., 2008). The parameters used in describing the temperature response were taken from Long & Bernacchi (2003).

Estimation of \( C_i \) and \( g_s \)

During the calculation of leaf photosynthesis, \( C_i \) and \( g_s \) were estimated using eqns (7)–(12) as in previous studies (Humphries & Long, 1995; Song et al., 2013) based on Ball et al. (1987). Equation (12) shows the calculation of intercellular CO\(_2\) partial pressure (\( C_i \), \( \mu \)bar) based on the CO\(_2\) partial pressure on the leaf surface (\( C_s \), \( \mu \)bar), photosynthetic CO\(_2\) assimilation rate (\( A \), \( \mu \)mol m\(^{-2}\) s\(^{-1}\)), stomatal conductance (\( g_s \), \( \mu \)mol m\(^{-2}\) s\(^{-1}\)) and air pressure (\( P_a \), bar). Equation (11) shows the calculation of CO\(_2\) partial pressure on the leaf surface (\( C_i \)) based on the ambient CO\(_2\) partial pressure (\( C_s \), \( \mu \)bar), photosynthetic CO\(_2\) assimilation rate (\( A \)), leaf boundary conductance (\( g_b \), \( \mu \)mol m\(^{-2}\) s\(^{-1}\)) and air pressure (\( P_a \)). The parameters \( a \), \( b \) and \( c \) calculated in eqns (8)–(10) are those used in eqn (7), which is an empirical equation used to calculate \( g_s \) based on the CO\(_2\) partial pressure on the leaf surface (\( C_i \)), photosynthetic CO\(_2\) assimilation rate (\( A \)), leaf boundary conductance (\( g_b \)), relative humidity (RH), partial pressure of the saturated water vapour for the air temperature (\( e_{air} \), mbar) and for leaf temperature (\( e_{leaf} \), mbar), stomatal coefficient \( g_b \) (20) and stomatal coefficient \( g_s \) (11.35). The equations used in this study to calculate stomatal conductance are suitable to model plants without water stress (Ball et al., 1987).

To adapt the Ball–Berry model to simulate plants under water stress conditions, additional factors associated with leaf water potential or soil water content are needed (Buckley et al., 2003; Li et al., 2012).

\[
g_s = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \tag{7}
\]

\[
a = C_s \tag{8}
\]

\[
b = -(g_0 \cdot C_s + 100g_1 \cdot A - C_s \cdot g_b) \tag{9}
\]

\[
c = -(100g_1 \cdot A \cdot RH \cdot e_{air} \cdot e_{leaf} \cdot g_b + g_0 \cdot C_s \cdot g_b) \tag{10}
\]

\[
C_s = C_a - \frac{A}{g_s} \cdot P_a \tag{11}
\]

\[
C_i = C_s - \frac{A}{g_s} \cdot P_a \tag{12}
\]

Temperature response of photosynthetic parameters

Leaf temperature affects photosynthetic parameters and eqns (13)–(21) were used to describe the temperature responses of photosynthetic parameters.

\[
\Theta = 0.76 + 0.018T - 3.7 \times 10^{-4}T^2 \tag{13}
\]

\[
\Gamma s = \exp(c_{I\Gamma s} - \Delta H_a,\Gamma s/RT_k) \tag{14}
\]

\[
C_i = 0.7C_s \cdot [(1.6740 - 6.1294 \cdot 10^{-3}T + 1.1688 \cdot 10^{-7}T^2 - 8.8741 \cdot 10^{-10}T^3)/0.73547] \tag{15}
\]

At 25 °C, \( C_i = 0.7C_s \)

\[
O_1 = 210(4.7000 \cdot 10^{-1} - 1.3087 \cdot 10^{-3}T + 2.5603 \cdot 10^{-6}T^2 - 2.1441 \cdot 10^{-9}T^3)/2.6934 \cdot 10^{-2} \tag{16}
\]

At 25 °C, \( O_{1 \mu} = O_a \)

\[
V_{c\max} = V_{c\max}0 \exp(c_{V_c\max} - \Delta H_a V_{c\max}/RT_k) \tag{17}
\]

\[
J_{\max} = J_{\max}0 \exp(c_{J_{\max}} - \Delta H_a J_{\max}/RT_k) \tag{18}
\]

\[
R_d = R_{d0} \exp(c_{R_d} - \Delta H_a R_d/RT_k) \tag{19}
\]

\[
K_o = \exp(c_{K_o} - \Delta H_a K_o/RT_k) \tag{20}
\]

\[
K_c = \exp(c_{K_c} - \Delta H_a K_c/RT_k) \tag{21}
\]

Iterative calculation of \( C_i \), \( g_s \) and \( P \) under constant leaf temperature

Equations (1)–(21) together form a system of equations, which was solved by using the Newton–Raphson method. During this computation, the initial \( C_i \) was calculated (eqn
Calculation of GPP

GPP was calculated by integrating the photosynthesis rates of all leaves in a canopy (eqn 22).

\[
GPP = \sum_{i} \frac{P_i \cdot S_i}{S_{\text{ground}}}
\]

where \( P_i \) is leaf photosynthesis rate for the \( i \)th leaf facet (the ‘\( i \)’ here is the sequence ID of a facet in the data file, ‘leaf ID’ is used to label a leaf for parameterization of leaf photosynthetic parameters) and \( S_i \) is the corresponding leaf area of the leaf facet. \( S_{\text{ground}} \) is the ground area occupied by the canopy.

To study GPP on different days during the growing season and to compare the whole season GPP of soybean under ambient and elevated CO\(_2\) conditions, the GPP per day or per season was calculated by integrating GPP during a day or throughout the growing season (eqn 23).

\[
GPP_{\text{day}} = \int_{t=1}^{24} P_{c,i} dt = \int_{t=1}^{24} \int_{u=0}^{3600} P_{c,i} du dt \approx \sum_{i=1}^{24} P_{c,i} \times 3600
\]

where \( GPP_{\text{day}} \) is the GPP per day, \( P_{c,i} \) is total canopy photosynthetic CO\(_2\) uptake for a unit ground area during a particular hour; \( P_{c,i} \) is total canopy photosynthetic CO\(_2\) uptake at the midpoint of an hour, i.e. at the 30th minute in each hour.

Cumulative GPP (cGPP) from the start day (168 DOY) to different days \( n \) between 168 DOY and 267 DOY was calculated by adding \( GPP_{\text{day}} \) from the start day to day \( n \) (eqn 24).

\[
cGPP(n) = \sum_{i=1}^{n} GPP_{\text{day},i} (168 \leq n \leq 267)
\]

Calculation of GPP under ambient and elevated CO\(_2\) conditions

The model was parameterized for both ambient and elevated CO\(_2\) conditions (Table 2). The parameters used include [CO\(_2\)], \( V_{\text{cmax}} \) and \( J_{\text{max}} \), air temperature and canopy structure on different days from 168 DOY to 267 DOY (for each day, the model was run three times).

Estimation of above-ground biomass from cGPP

Model-estimated above-ground biomass was calculated based on cGPP, the harvest index, carbon content in different organs and root : shoot ratio. Briefly, we first calculated the total carbon in biomass \( (W_c) \) by subtracting respiration from cGPP assuming that respiration is 57.5 % of total photosynthetic CO\(_2\) uptake (Amthor, 2000). Second, the proportion of carbon for the whole plant was calculated based on the harvest index, the proportion of carbon in pod and seed, and the proportion of carbon in other parts of the soybean, which was assumed as \((C\ H\mathrm{_{10}}\ O_5)\). We assumed that the composition of soybean pod and seed was carbohydrate (29 %), protein (37 %), lignin (6 %), organic acid (5 %) and mineral (5 %); this results in a proportion of carbon \((C\ H\mathrm{_{10}}\ O_5)\) of 53 % in pod and seed (Amthor, 2000). We also assumed that the composition of root, stem and leaf biomass was \((C\ H\mathrm{_{10}}\ O_5)\), which results in a proportion of carbon \((C\ H\mathrm{_{10}}\ O_5)\) being 44.4 %. We further assumed a harvest index \( \eta \) of 0.57 (Pedersen & Lauer, 2004; Spaeth et al., 2010), and then calculated the proportion of carbon in a whole soybean plant \((C_{\text{plant}})\) as:

\[
C_{\text{plant}} = C_{\text{pod+seed}} \cdot \eta + C_{\text{other}} \cdot (1 - \eta)
\]

Whole plant biomass was given by:

\[
BM_{\text{total}} = \frac{W_c}{C_{\text{plant}}}
\]

Finally, assuming a ratio of root to total biomass \((p_{\text{root}})\) as 18.7 % (Clough & Peet, 1981), we calculated above-ground biomass:

\[
aBM = BM_{\text{total}} \cdot p_{\text{root}}
\]

Dissecting the factors contributing to changes in GPP under elevated CO\(_2\)

To evaluate the relative contribution of physiological parameters (i.e. \( V_{\text{cmax}} \) and \( J_{\text{max}} \)), architectural parameters and environmental factors (i.e. air temperature and CO\(_2\)) to the changed GPP under elevated CO\(_2\), we simulated GPP under different scenarios. The method was adapted from the sensitivity analysis of a model that is commonly used in previous studies (Zhu et al., 2007; Wu & Cournède, 2010). The different scenarios are listed in Table 3. The contribution of all four factors, i.e. CO\(_2\) \( (C)\), canopy structure \( (S)\), temperature \( (T)\), and \( V_{\text{cmax}} \) and \( J_{\text{max}} \) \( (V)\) can be split into the contribution of single factors \( c(C)\), \( c(S)\), \( c(T)\) and \( c(V)\), interactions between two factors \( c(CS)\), \( c(CT)\), \( c(CV)\), \( c(ST)\), \( c(SV)\) and \( c(TV)\), interactions between three factors \( c(CST)\), \( c(CSV)\), \( c(CTV)\) and \( c(STV)\), and interaction between four factors \( c(CSTV)\) as shown in eqn (28). The contribution of any single factor \( c(X)\) was calculated from eqn (29); the contribution of an interaction of any two factors \( c(XY)\) is calculated from eqn (30).
Table 3. Scenarios used to calculate GPP, which is used to dissect the contributions of individual factors ([CO₂], V_{cmax} and J_{max}, T, canopy structure) and their interactions to changes in GPP

| Scenarios | Elevated CO₂ (X), Ambient CO₂ (–) | [CO₂] | V_{cmax} J_{max} | T | Canopy structure |
|-----------|----------------------------------|-------|-----------------|---|-----------------|
| O         | – – –                            | –     | – –             | – | –               |
| C         | X – –                            | –     | – X             | – | –               |
| V         | – X –                            | –     | X –             | – | –               |
| T         | – – X                            | –     | – X             | – | –               |
| S         | – – –                            | –     | – X             | – | –               |
| C,V       | X X –                            | –     | – X             | – | –               |
| C,T       | X X –                            | –     | X –             | – | –               |
| C,S       | X – –                            | –     | – X             | – | –               |
| V,T       | X X –                            | –     | – X             | – | –               |
| V,S       | – X X                            | –     | X –             | – | –               |
| T,S       | – – X                            | –     | – X             | – | –               |
| C,V,T     | X X X                            | –     | – X X           | X | –               |
| C,V,S     | X X X                            | –     | X –             | – | –               |
| C,T,S     | X X X                            | –     | – X X           | X | –               |
| V,T,S     | X X X                            | –     | X –             | – | –               |
| C,V,T,S   | X X X                            | –     | X –             | – | –               |

A dash (‘–’) represents a factor under ambient CO₂ conditions, and ‘X’ represents a factor under elevated CO₂ conditions. The scenarios include all the combinations of four factors, i.e. [CO₂], V_{cmax} and J_{max}, air temperature (T) and canopy structure, under two conditions, i.e. elevated [CO₂] and ambient [CO₂].

was calculated from eqns (29) and (30); and the contribution of an interaction among any three factors c(XYZ) was calculated from eqns (29–31). In this study, the relative contributions of each factor and the interactions between factors were calculated by solving a system of linear equations where c(X), c(XY), c(XYZ) and c(CSTV) are variables.

\[
GPP(X,Y,Z) - GPP(O) = c(X) + c(Y) + c(Z) + c(XZ) + c(YZ) + c(XY) + c(XYZ) + c(STV) + c(CSTV) + c(CSV) + c(CTV) + c(CSTV)
\]

(28)

\[
GPP(X) - GPP(O) = c(X)
\]

(29)

\[
GPP(X,Y) - GPP(O) = c(X) + c(Y) + c(XY)
\]

(30)

\[
GPP(X,Y,Z) - GPP(O) = c(X) + c(Y) + c(Z) + c(XY) + c(XZ) + c(YZ) + c(XYZ)
\]

(31)

Statistical analysis

Pearson’s correlation coefficient was calculated with the R software function cor. Student’s t-test was calculated with the R software function t.test.

RESULTS

Canopy architectural and physiological data used to develop soybean canopy models

Soybean grown under elevated [CO₂] revealed about a 10–90 % increase in leaf area and leaf width for different leaves (Supplementary Data Tables S1 & S2). Leaf angle distributions were assumed to be the same for both CO₂ treatments based on field observations (Table S3). Internode distances were obtained from direct measurements under ambient [CO₂] conditions (Table S4). Internode distances for soybean grown under elevated [CO₂] were 6 % longer than under ambient [CO₂] conditions (Ainsworth et al., 2002). The probabilities of node numbers of the main stem and branches at the final stage were assumed to be the same between the two [CO₂] conditions and were measured (Table S5). For the main stem, all measured plants had more than ten nodes; 95 % of plants had more than 11 nodes; with an increase in node number, the percentage of plants having more than the node number gradually decreased (Table S5). Node probabilities differed dramatically between branches. For example, the probability of having more than one node was 10 % for Br1, 50 % for Br2 and 30 % for Br3 (Table S5). Maximal node numbers of the main stem and different branches during a growing season under ambient and elevated [CO₂] conditions are given in Tables S6 and S7, which was compiled based on a previous study (Castro et al., 2009). Growth of the main stem and branch was faster under elevated [CO₂] than under ambient [CO₂] (Tables S6 and S7). We used the number of leaves defoliated from stands to quantify leaf senescence. Leaves senesced faster under elevated [CO₂] than under ambient [CO₂] (Table S8). Leaf photosynthetic parameters, V_{cmax} and J_{max}, collected based on Bernacchi et al. (2005), are shown in Table S9.

GPP during a growing season under elevated and ambient CO₂ conditions

Simulated GPP_{dry} was higher under elevated [CO₂] compared to ambient [CO₂] throughout the growing season (Fig. 2A), with the relative increase in simulated GPP_{dry} being higher in the early growth season (DOY<200) (Fig. 2B). The seasonal trends in simulated daily GPP (GPP_{dry}) mimicked the behaviour of measured LAI with an initial fast increase, followed by a peak in GPP_{dry} near the date of peak LAI and a final decline towards the end of the growing season (Fig. 2A, C). Simulated cGPP showed a high degree of correlation (Pearson coefficient > 0.99) with measured aBM (Morgan et al., 2005), under both ambient and elevated [CO₂] conditions (Fig. 2D) (Supplementary Data Table S10). To compare the model simulation with measured data, we further estimated the above-ground biomass with cGPP. The model-estimated above-ground biomass was linearly correlated with measured values, with slope being 0.96 and 0.97 under elevated and ambient CO₂, respectively (Fig. 2E). The R² values for these two relationships were 0.995 and 0.992 for elevated and ambient CO₂ respectively (Fig. 2E).

Contributions of CO₂ concentration, canopy structure, leaf temperature and V_{cmax} and J_{max} to the increase of GPP under elevated [CO₂]

Between soybean plants grown under elevated [CO₂] and ambient [CO₂], four factors (i.e. CO₂ concentration, temperature, V_{cmax} and J_{max}, and canopy structure, which includes leaf size and leaf number) differed (Table 2). Here we used canopy photosynthesis models to dissect the contribution of each of these
factors, and their interactions, to increase GPP in elevated [CO₂] compared to ambient [CO₂] (ΔGPP) (Fig. 3). Figure 3A shows the averaged contributions over the growing season of CO₂ (76.7 %), canopy structure (17.2 %) and their interaction (2.6 %) to increases in ΔGPP (Fig. 3A). The increase in air temperature under elevated CO₂ showed a mild negative impact (−0.1 %) on ΔGPP, but the interaction between CO₂ and temperature showed a substantial positive impact (6.9 %) on ΔGPP (Fig. 3A). Vₖₐₓ and Jₖₐₓ negatively influenced ΔGPP, i.e. decreasing GPP by −6.7 % of ΔGPP, but their interactions with CO₂ had a positive impact of 3.3 % on AGPP (Fig. 3A). The contributions of other interactions on ΔGPP are not significant (<1 %) (Fig. 3A).

To further investigate the impacts of these factors on ΔGPP in different growth stages and weather conditions, we chose a Sunny day in the Early developmental stage (SE), a Cloudy day in the Late developmental stage (CL), and a Sunny day at a Later developmental stage (SL) for analysis (Fig. 3B–D). The contribution of CO₂ concentration was smaller in SE (62.5 %) than in SL (99.8 %) and the contribution of canopy structure was greater in CL (6 %) than in SL (4.8 %) (Fig. 3C, D).
Canopy absorbance and PPFD distribution in different stages and weather conditions

To explore the greater relative contribution of canopy structure to \( \Delta \text{GPP} \) in the earlier growth stages, we analysed the canopy absorbance for SE, SL and CL days (Fig. 4). In the earlier stages, canopy absorbance decreased with time in the morning and increased in the afternoon because the canopy was not closed to fully cover the ground (LAI = 2.6 for ambient and 2.9 for elevated [CO\(_2\)]), resulting in more light penetrating through the canopy and reaching the soil surface when solar elevation angle increased (Fig. 4B). In later growth stages, canopy absorbance was relatively constant over the course of a day (Fig. 4E, H). The difference in daily averaged canopy absorbance between the two [CO\(_2\)] conditions was larger in SE (6.2 \%) than SL (1.2 \%) and CL (1.0 \%) (Fig. 4C, F, I).

The PPFD distribution in SE was more uniform than in SL (Fig. 5A, D). The canopy in SL experienced more scattered PPFD or sunflecks in the bottom layers than that in CL (Fig. 5D, G). The light extinction coefficients for canopies developed under elevated [CO\(_2\)] and ambient [CO\(_2\)] were almost the same in either SL, CL or SE days (Fig. 5B, E, H). With increasing cLAI, canopy absorbance increased but did not saturate in SE, increased and approached saturation at about cLAI = 6 in SL, and increased and approached saturation at about cLAI = 3 in CL. The marginal canopy absorbance, defined as \( \frac{d(\text{Abs})}{d(\text{cLAI})} \), was much higher (0.24) in SE, comparing to those at the later stages (0.04 for SL and 0.02 for CL) (Fig. 5C, F, I).

Synergistic effect of PPFD on the contribution of [CO\(_2\)] to \( \Delta \text{GPP} \)

For mature canopies (DOY > 207), daily \( \Delta \text{GPP}_{\text{CO}_2} \) was positively correlated (\( R^2 = 0.727 \)) with the daily averaged ambient solar PPFD (Fig. 6A). In Fig. 6A, diurnal average PPFD is the diurnal averaged ambient solar PPFD, while points represent PPFD of different days of the later developmental stages. For these days, we also calculated \( \Delta \text{GPP} \) contributed by elevated [CO\(_2\)], and found that on days with high ambient PPFD (i.e. sunny days), ‘\( \Delta \text{GPP} \) contributed by elevated CO\(_2\)’ was higher; on days with low ambient PPFD (i.e. cloudy days), the ‘\( \Delta \text{GPP} \) contributed by elevated CO\(_2\)’ was lower. Although daily GPP is a function of daily total intercepted solar radiation, here we used the average ambient PPFD as the \( x \)-axis to ease comparison with Fig. 6B, which shows the simulated light response curves of leaf photosynthetic CO\(_2\) uptake rate (AQ curve) for both ambient and elevated CO\(_2\) conditions on 219 DOY (Fig. 6B) (data of AQ curves for 210–252 DOY are given in Supplementary Data Table S11). When PPFD was lower than about 800 \( \mu \text{mol} \, \text{m}^{-2} \, \text{s}^{-1} \) and photosynthesis was limited by RuBP regeneration, the increase in leaf photosynthesis rate (\( \Delta \text{P} \)) was about 11 \% under elevated CO\(_2\) compared to ambient CO\(_2\) condition (Fig. 6B). When PPFD was greater than 800 \( \mu \text{mol} \, \text{m}^{-2} \, \text{s}^{-1} \)
and photosynthesis was limited by Rubisco, $\Delta P$ was as high as 24\% (Fig. 6B).

DISCUSSION

This study presents a new integrative framework that coupled an explicit 3-D soybean architecture model with a ray tracing algorithm (Song et al., 2013) and a leaf photosynthesis model (Farquhar et al., 1980; Ball et al., 1987; Monteith & Unsworth, 2007) to compute whole canopy photosynthetic response under different environments. In addition, the integrated model also incorporated the responses of photosynthetic parameters to temperature (Bernacchi et al., 2001, 2003). The integrated model was employed in this study to dissect the contribution of different factors to the changes in GPP of soybean grown under elevated [CO$_2$]. Model simulations over the entire growing season demonstrated that CO$_2$ fertilization and structural acclimation significantly increased whole canopy $\Delta$GPP, while photosynthetic acclimation and leaf temperature changes played a minor effect (Fig. 3). Furthermore, we show that the impacts of these different factors on the observed $\Delta$GPP varied with different canopy architecture parameterizations and weather conditions (Fig. 3). Finally, we demonstrate a synergistic effect of CO$_2$ and light on $\Delta$GPP. Specifically, an increase in LAI under elevated [CO$_2$] during the early developmental stage dramatically increased light absorption and hence canopy photosynthesis (Figs 4 and 5); at later developmental stages, on days with high ambient light (i.e. on bright sunny days), the contribution of elevated CO$_2$ to GPP was larger than that under lower ambient light (i.e. on cloudy days), because the proportion of leaves in a canopy undertaking Rubisco-limited photosynthesis increased when ambient PPFD increased (Fig. 6).

A new method to dissect the contribution of different factors and their interactions to $\Delta$GPP

This study used the canopy architectural parameters for each developmental stage to construct 3-D canopy models along the growing season (Fig. 1). This enabled quantification of GPP for plants at each developmental stage (Fig. 2A, B). Previous studies have used the sunlit–shaded model to simulate light environments inside the canopy and canopy photosynthesis (DePury & Farquhar, 1997; Wang & Leuning, 1998). In this study, we applied a ray tracing algorithm coupled with
3-D canopy architecture model to simulate the fine details or heterogeneities of light environments in the soybean canopies (Fig. 5A, D, G).

Another major feature of the model was the 3-D canopy photosynthesis model along the growing season. In some previous studies, 3-D canopy photosynthesis models have been built for a
particular developmental stage (Zheng et al., 2008; Song et al., 2013; Pound et al., 2014). Here we developed a routine to extrapolate the architectural parameters along the whole growth cycle using architectural parameters measured in a representative developmental stage. Our method uses probability tables to randomize node numbers on the main stem and branches (Supplementary Data Tables S5 and S6). The senescence of soybean leaves begins from the bottom of a canopy, with senescent leaves dropping to the ground causing a decrease in LAI at later developmental stages (Setiyono et al., 2008). Such leaf senescence has been modelled by decreasing the LAI (Yin, 2000). In this study, we modelled the number of senescent leaves with a probability table and those senesced leaves was removed directly from the 3-D canopy model (Table S8; Fig. 1).

The model-calculated GPP was linearly correlated with the measured above-ground biomass (Morgan et al., 2005) along the growing season, and the obtained coefficient of determination, $R^2$, was higher than 0.99 (Fig. 2D), which suggests that the model can be used to study factors influencing variations of GPP and hence biomass production. Assuming a fixed root : shoot ratio (Ainsworth et al., 2002) and a fixed fraction of dark respiration (Amthor et al., 2001), the model predicted a 21.4 % increase in above-ground biomass when increasing [CO$_2$] from 370 to 550 ppm (Fig. 2; Supplementary Data Table S10). Our model prediction is largely consistent with results from earlier studies. Previous studies showed that when [CO$_2$] is increased to about 700 ppm, total biomass increases by about 37 % (Ainsworth et al., 2002); when [CO$_2$] is increased to about 550 ppm, above-ground biomass increases by about 17–18 % (Morgan et al., 2005). The difference between the measured and predicted increase in biomass can be attributed to a number of factors: difference between the predicted vs. measured $V_{\text{max}}$ and $J_{\text{max}}$ for leaves at different layers of a canopy, and potential heterogeneity of microclimatic factors other than light (e.g. CO$_2$, humidity) inside canopies. These areas need to be improved in future canopy photosynthesis modelling studies.

**Dissection of the contribution of different factors to $\Delta$GPP**

This model provides a unique opportunity to dissect the contribution of different factors to changes in GPP ($\Delta$GPP) under elevated [CO$_2$] as compared to that under ambient [CO$_2$]. The CO$_2$ fertilization effect showed the greatest contribution (76.7 %), followed by canopy architecture (17.2 %), to $\Delta$GPP (Fig. 3A). This dominant role of elevated [CO$_2$] to $\Delta$GPP is consistent with an earlier study which showed that changes in the canopy photosynthetic energy conversion efficiency contributed 80 % and the interception efficiency contributed 20 % to the increase in soybean yield under elevated [CO$_2$] (Dermody et al., 2008). The contribution of canopy structure, as shown in the present study, can be further divided into the contribution of LAI and contribution from architecture. LAI directly determines the total photosynthesis leaf area and greatly influences canopy photosynthesis (Song et al., 2013). In this study, the leaf size of soybean was 1.1–1.9 times larger under elevated [CO$_2$] than under ambient [CO$_2$] depending on the growth stages (Supplementary Data Tables S1 and S2). The architecture of the canopy was not changed under elevated [CO$_2$] compared with ambient [CO$_2$].

Changes in leaf temperature showed a minor influence (~0.1 %) on $\Delta$GPP. Temperature can influence a number of factors related to $\Delta$GPP. First, it influenced leaf photosynthetic rates. In SoyFACE, the soybean growth temperature was around the optimal temperature for soybean leaf photosynthesis (Supplementary Data Fig. S1), which was reported to be at about 28 °C based on the temperature response to photosynthesis (Bernacchi et al., 2001, 2003; Medlyn et al., 2002). A further increase in leaf temperature in SoyFACE decreased canopy photosynthesis. Second, temperature can alter leaf respiration. In a previous study, the negative impact of temperature on rice yield has been attributed to increased respiration at night (Peng et al., 2004). Increased leaf temperature can increase leaf respiration rate, which is usually modelled via the Q10 parameter. Note that total canopy respiration is usually positively correlated with LAI and canopy total nitrogen content. LAI increased by about 19 % under elevated [CO$_2$] to increase in total canopy respiration; however, the leaf nitrogen content on a leaf area basis decreases by an average of 3.9 % in crops under elevated [CO$_2$] as result of Rubisco acclimation (Leakey et al., 2009).

Under elevated [CO$_2$] conditions, while Rubisco content decreases by 19 %, $V_{\text{max}}$ at 25 °C decreases only by 15 % due to increased Rubisco activation state (Ainsworth & Long, 2005). The photosynthetic acclimation to growth under elevated [CO$_2$] observed in later developmental stages under the elevated [CO$_2$] condition increases the nitrogen use efficiency of the photosynthesis system (Long et al., 2004) and contributed to $\Delta$GPP by about ~6.7 % (Fig. 3).

Synergistic effect of CO$_2$ and light on $\Delta$GPP

This study reveals a synergetic effect of CO$_2$ and light on $\Delta$GPP. On the one hand, elevated CO$_2$ promoted photosynthesis and growth of the plant canopy, which resulted in a higher LAI. The higher LAI led to more light absorption, which increased canopy photosynthesis. At early developmental stages, when LAI was relatively low, canopy absorbance under elevated [CO$_2$] can be 6.2 % higher than that under ambient [CO$_2$] (Fig. 4C). This positive effect of LAI on light absorbance decreased with increasing LAI; at later developmental stages, the difference in canopy absorbance between canopies grown under elevated vs. ambient [CO$_2$] was only about 1–1.2 % because the canopy intercepted about 90 % of total PPFD when LAI > 6 (Fig. 5F, I). The increase in leaf area under elevated CO$_2$ can increase canopy respiration, which decreased the positive impact of increasing LAI on net canopy photosynthesis. In fact, greater than optimal LAI can even lead to decreased canopy photosynthesis (McCree & Troughton, 1966; Anten et al., 1995; Song et al., 2013).

The synergistic effect between CO$_2$ and light on $\Delta$GPP is shown by the correlation between daily averaged PPFD and $\Delta$GPP (Fig. 6A), which shows that the impact of elevated [CO$_2$] on $\Delta$GPP was positively correlated with ambient PPFD. Canopy photosynthetic rate is the integral of photosynthetic rates of all leaves in a canopy. Every facet of the every leaf in a canopy is under either Rubisco limitation or RuBP-regeneration limitation depending on its photosynthetic parameters and the absorbed PPFD. The proportion of leaves in
which photosynthesis is limited by Rubisco is higher on sunny days than on cloudy days. CO₂ can influence photosynthesis through two mechanisms, i.e. suppressing photorespiration and increasing substrate availability to Rubisco (Long et al., 2004). When photosynthesis was limited by RuBP regeneration, leaf photosynthetic rate under a [CO₂] of 550 ppm was 11% higher than that under a [CO₂] of 370 ppm, mainly due to suppression of photorespiration (at low light in Fig. 6B); in contrast, when photosynthesis was limited by Rubisco, a potential 24% increase in leaf photosynthetic rate was predicted as a result of both suppressing photorespiration and increased substrate availability for Rubisco (at high light in Fig. 6B). Therefore, with an increase in ambient PPFD, the proportion of leaves under Rubisco-limited photosynthesis increases from 12.2% under low PPFD to 35.6% under high PPFD (Supplementary Data Fig. S2), which leads to an increased contribution of elevated CO₂ on canopy photosynthesis or AGPP.

CONCLUSION

We integrated an existing 3-D canopy photosynthesis model (Song et al., 2013) with data describing the architectural and physiological changes of soybean grown under ambient and elevated CO₂ conditions. Table S2: Leaf length of soybean in the mature stage under both ambient and elevated CO₂ conditions. Table S2: Leaf width of soybean in the mature stage under both ambient and elevated CO₂ conditions. Table S3: Branch angle, petiole angle, mid-leaf angle and leaf angles of leaf, middle and right leaves in a trifoliate leaf in the mature stage used for parameterization of the soybean architecture models under both ambient and elevated CO₂ conditions. Table S4: Internode and petiole lengths for each node in the main stem and those for branches used for parameterization of the canopy architecture model under both ambient and elevated CO₂ conditions. Table S5: Probabilities of node numbers for the main stem and the branches used for parameterization of the canopy architecture model under both ambient and elevated CO₂ conditions. Table S6: Maximal node numbers of the main stem and the branches for Br1 to Br2 of soybean under ambient and elevated CO₂ conditions. Table S7: Maximal node numbers of the main stem and branches for Br3 to Br6 of soybean under ambient and elevated CO₂ conditions. Table S8: Senescence leaf numbers in every 3 d for soybean grown under ambient and elevated CO₂ conditions. Table S9: Vmax and Jmax for top leaves of soybean grown under ambient and elevated CO₂ conditions during a growing season. Table S10: Biomass, model-calculated cumulative GPP. Table S11: Leaf photosynthesis at different PPFD under both ambient and elevated [CO₂] conditions. Figure S1: Air temperature, relative humidity and photosynthetic photon flux density during the growing season from 168 DOY to 267 DOY used for modelling canopy photosynthesis. Figure S2: The proportion of Rubisco-limited photosynthesis under high light and under low light.

Supplementary data are available online at https://academic.oup.com/aob and consist of the following. Table S1: Leaf length of soybean in the mature stage under both ambient and elevated CO₂ conditions. Table S2: Leaf width of soybean in the mature stage under both ambient and elevated CO₂ conditions. Table S3: Branch angle, petiole angle, mid-leaf angle and leaf angles of leaf, middle and right leaves in a trifoliate leaf in the mature stage used for parameterization of the soybean architecture models under both ambient and elevated CO₂ conditions. Table S4: Internode and petiole lengths for each node in the main stem and those for branches used for parameterization of the canopy architecture model under both ambient and elevated CO₂ conditions. Table S5: Probabilities of node numbers for the main stem and the branches used for parameterization of the canopy architecture model under both ambient and elevated CO₂ conditions. Table S6: Maximal node numbers of the main stem and the branches for Br1 to Br2 of soybean under ambient and elevated CO₂ conditions. Table S7: Maximal node numbers of the main stem and branches for Br3 to Br6 of soybean under ambient and elevated CO₂ conditions. Table S8: Senescence leaf numbers in every 3 d for soybean grown under ambient and elevated CO₂ conditions. Table S9: Vmax and Jmax for top leaves of soybean grown under ambient and elevated CO₂ conditions during a growing season. Table S10: Biomass, model-calculated cumulative GPP. Table S11: Leaf photosynthesis at different PPFD under both ambient and elevated [CO₂] conditions. Figure S1: Air temperature, relative humidity and photosynthetic photon flux density during the growing season from 168 DOY to 267 DOY used for modelling canopy photosynthesis. Figure S2: The proportion of Rubisco-limited photosynthesis under high light and under low light.

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