Modelling equations used in Figure 4

Here we derive the key equations used in Figures 4 to calculate CO_2 assimilation rate, A, chloroplast CO_2 partial pressure, $C_{chlo,}$ from Rubisco and bicarbonate transporter activities and cell wall/plasamalema conductance, g_w and chloroplast envelope conductance, g_{chlo} to CO_2 diffusion. The equations are based on the C_4 and C_3 photosynthetic models given in von Caemmerer and Furbank (1999) and von Caemmerer (2000) and have been adapted from the single cell C_4 photosynthesis model presented by von Caemmerer and Furbank (2003).

CO_2 assimilation rate of a hypothetical C_3 photosynthesis system with a bicarbonate pump at the chloroplast envelope outlined in Figure 3a and 4 can be described by two simple equations. Since ultimately all CO_2 is fixed by Rubisco in the chloroplast the net rate of CO_2 assimilation, A, is

$$A = V_c - 0.5V_o - R_d \qquad \text{(A1)}$$

where V_c and V_o are the rates of Rubisco carboxylation and oxygenations and R_d is the rate of mitochondrial respiration not associated with photorespiration.

We assume that the chloroplast receives extra CO_2 from the from the transport of bicarbonate into the chloroplast, such that

$$V_c = V_b - L \qquad \text{(A2)}$$

where V_b is combined rate of the bicarbonate transporters, and L is the rate of CO_2 leakage across the chloroplast envelope. Equation (A2) differs from the standard formulation of the C_4 model because we assume that photorespiratory CO_2 loss occurs in the cytosol compartment. The leakage L in turn is given by

$$L = g_{chlo}(C_{chlo} - C_{cyt}) \qquad \text{(A3)}$$

Where C_{chlo} and C_{cyt} are the chloroplast and cytosol CO_2 partial pressures respectively. Leakiness, ϕ, can then be defined as the leak rate as a fraction of the rate of bicarbonate transport.

$$\phi = L/V_b \qquad \text{(A4)}$$

It should be noted that leakrate and leakiness will be positive only if C_{chlo} is greater than $C_{cyt.}$ At high irradiance the maximal activity of Rubisco limits the rate of CO_2 fixation rather than the light dependent capacities for the regeneration of RuBP which is not considered here.

Under these conditions Rubisco carboxylations is given by the RuBP saturated rate

$$V_c = \frac{C_{chlo} V_{c\max}}{C_{chlo} + K_c (1 + O \ / K_o)} \tag{A5}$$

where V_{cmax} is the maximum carboxylation rate and K_c and K_o are the Michaelis-Menten constants for CO_2 and O_2 and O is the O_2 partial pressure in the chloroplast. Following the oxygenation of one mol of RuBP, 0.5 mol of CO_2 is evolved in the photorespiratory pathway. The ratio of oxygenation to carboxylation can be expressed as

$$V_o / V_c = 2 \Gamma_* / C_{chlo} \tag{A6}$$

and Γ_* the CO_2 compensation point in the absence of mitochondrial respiration is determined by Rubisco's specificity ($S_{c/o}$):

$$\Gamma_* = \frac{0.5 O}{S_{c/o}} = 0.5 [V_{o\max} K_c / (V_{c\max} K_o)] O \tag{A7}$$

where V_{omax} is the maximal oxygenase activity.

The rate of bicarbonate transport is given as

$$V_b = \frac{C_{\mathrm{cyt}} V_{b\max}}{C_{\mathrm{cyt}} + K_b} \tag{A8}$$

where V_{bmax} is the maximal activity of the transporter and K_b is the Michaelis Menten constant for CO_2. This was converted from the Michaelis Menten constant for bicarbonate with the use of the Henderson Hasselbach equation assuming a cytosolic pH of 7.4. If more than one transporter is involved the individual rates can be summed. We modelled the rate of BicA (V_{bic}) and SbtA (V_{Sb}) individually and combined.

To obtain an overall rate equation for CO_2 assimilation as a function of the cytosol CO_2 partial pressure one can first derive a quadratic expression for the chloroplast CO_2 partial pressure C_{chlo}, by combining equations A2, A3 and A5.

This gives a quadratic of the form

$$(C_{chlo})^2 + b(C_{Chlo}) \ + c = 0 \qquad \text{(A9)}$$

where

$$C_{chlo} = \left(-b + \sqrt{b^2 - 4c}\right)/(2) \qquad \text{(A10)}$$

and

$$b = -\left\{C_{cyt} - K_c(1 + O/K_o) + (V_b - V_{c\max})/g_{chlo}\right\} \qquad \text{(A11)}$$

$$c = -K_c(1 + O/K_O)(C_{cyt} - V_b/g_{chlo}) \qquad \text{(A12)}$$

With a solution for $C_{chlo,}$ A can be calculated form equations A1, A5, and A6. Intercellular CO_2, C_i, was calculated retrospectively from

$$C_i = C_{cyt} + A/g_w \qquad \text{(A13)}$$

where g_w is the conductance to CO_2 diffusion across the cell wall plasmalemma interface.

ATP consumption rate was calculated from

$$ATPconsumption = \alpha V_b + (3 + 7\,\Gamma_*/C_{chlo})V_c \qquad \text{(A14)}$$

(See equation 4.27 von Caemmerer 2000). The energy cost of bicarbonate transport is uncertain but we assumed that the bicarbonate transporter BicA required the transport of one H^+ whereas SbtA required 2 H^+. Assuming a requirement of 4 H^+ to generate an ATP we have calculated the ATP requirement of the transporters as 0.25ATP and 0.5 ATP per transport event respectively.

Supplementary Table 1 Photosynthetic parameters used in the model simulation

Parameter	Value
K_c (μbar)	260[a]
K_o (mbar)	179[a]
$S_{c/o}$ (bar/bar)	2585
Γ_* at 200 mbar O_2 (μbar)	38.6 [a]
V_{cmax} (μmol m^{-2} s^{-1})	100
R_d (μmol m^{-2} s^{-1})	0
V_{BicA} (μmol m^{-2} s^{-1})	30
K_{BicA} (μbar)	140
V_{SbtA} (μmol m^{-2} s^{-1})	15
K_{Sbta} (μbar)	15

[a] (von Caemmerer et al., (1994)).