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e-photosynthesis: a comprehensive dynamic mechanistic model of C₃ photosynthesis: from light capture to sucrose synthesis

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ABSTRACT

Photosynthesis is arguably the most researched of all plant processes. A dynamic model of leaf photosynthesis that includes each discrete process from light capture to carbohydrate synthesis, *e*-photosynthesis, is described. It was developed by linking and extending our previous models of photosystem II (PSII) energy transfer and photosynthetic C₃ carbon metabolism to include electron transfer processes around photosystem I (PSI), ion transfer between the lumen and stroma, ATP synthesis and NADP reduction to provide a complete representation. Different regulatory processes linking the light and dark reactions are also included: Rubisco activation via Rubisco activase, pH and xanthophyll cycle-dependent non-photochemical quenching mechanisms, as well as the regulation of enzyme activities via the ferredoxin-thioredoxin system. Although many further feedback and feedforward controls undoubtedly exist, it is shown that *e*-photosynthesis effectively mimics the typical kinetics of leaf CO₂ uptake, O₂ evolution, chlorophyll fluorescence emission, lumen and stromal pH, and membrane potential following perturbations in light, [CO₂] and [O₂] observed in intact C₃ leaves. The model provides a framework for guiding engineering of improved photosynthetic efficiency, for evaluating multiple non-invasive measures used in emerging phenomics facilities, and for quantitative assessment of strengths and weaknesses within the understanding of photosynthesis as an integrated process.

Key-words: ATPase; chlorophyll fluorescence quenching; cytochrome b₆f; phenomics; photoprotection; photorespiration; Rubisco activase; Rubisco; systems biology; thioredoxin.

INTRODUCTION

Farquhar, Von Caemmerer & Berry (1980) developed a steady-state mechanistic model of C₃ leaf photosynthetic carbon assimilation rate (*A*), which was subsequently modified (Harley & Sharkey 1991). This model reasons that *A*, under any given set of conditions, will be limited by the slowest of three processes: (1) the maximum rate of ribulose biphosphate carboxylase/oxygenase (Rubisco) catalysed

ribulose 1,5-bisphosphate (RuBP) carboxylation (Rubisco limited); (2) the regeneration of RuBP controlled by electron transport rate or enzymes in the C₃ cycle other than Rubisco (RuBP regeneration limited); and (3) the regeneration of RuBP controlled by the rate of triose-phosphate utilization (TPU limited). This model has been widely validated in predicting steady-state *A* under different environmental conditions (Beadle & Long 1985; Harley & Sharkey 1991; Harley *et al.* 1992; von Caemmerer 2000). However, photosynthesis is rarely at steady state in the natural environment due to fluctuating conditions of light, temperature, vapour pressure deficit, and other conditions, as well as feedbacks within the leaf. Furthermore, without explicit representation of each enzyme in photosynthesis, the Farquhar *et al.* (1980) model cannot alone be used to predict the impact of manipulating different genes and their protein products on *A*.

In terms of total global food production, wheat, rice and soybean are the major C₃ crops. It has become increasingly recognized that breeding of these crops has reached a point where further improvement of the potential yield is limited by photosynthetic capacity (Furbank *et al.* 2009; Long & Ort 2010; Zhu, Long & Ort 2010; Parry *et al.* 2011). The goal of identifying molecular targets to improve photosynthetic efficiency under field conditions as a means to improve crop yield would be significantly advanced by a comprehensive dynamic model of photosynthesis that includes as many photosynthesis-related reactions as possible (Zhu *et al.* 2010). The control of system flux in photosynthesis, which involves a complex series of interlinked biophysical and biochemical reactions, shifts among different reactions under different environmental conditions. Highly mechanistic, well-validated mathematical models of photosynthesis offer a practical means to select and prioritize among the multitude of potential permutations of targets for modification in engineering improved photosynthetic performance. This goal that has gained added importance as means other than photosynthesis in improving the potential yield of crop germ plasm are nearly exhausted (Long *et al.* 2006; Zhu, Long & Ort 2008; Zhu *et al.* 2010).

A comprehensive model of photosynthesis should include not only the individual steps, but also the major regulatory mechanisms affecting these steps, for example, the luminal pH (Kramer, Sacksteder & Cruz 1999), the redox state of the plastoquinone pool in the thylakoid membrane (Stirbet,

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Strasser & Strasser 1998), stromal pH (Martin, Scheibe & Schnarrenberger 2000), the redox state of thioredoxin (Schurmann & Jacquot 2000), its target enzymes (Hutchison *et al.* 2000) and the concentrations of key ions in the stroma and thylakoid lumen (Martin *et al.* 2000). Such an intricate model requires considerable computational power and advanced numerical algorithms to solve the resulting system of differential equations. This is especially so since the component reactions act on time scales that vary by orders of magnitude resulting in a stiff system of differential equations with respect to numerical integration (Zhu, De Sturler & Long 2007; Zhu *et al.* 2005). Algorithms have now been developed to deal with these stiff systems. These include variable order solvers that significantly improve computational efficiency (Shampine & Reichelt 1997; Shampine, Reichelt & Kierzenka 1999) and make it now possible to build a more complete model of photosynthesis than had been possible previously. The coalescence of an advanced knowledge about photosynthetic mechanisms, expanded computational power and efficient numerical integration algorithms provided this new opportunity to develop *e*-photosynthesis, the model presented here, as a quantitative framework for assessing knowledge and properties of the overall system.

Historically, mathematical models of photosynthesis with different levels of detail have been developed and used to test different hypotheses (Hahn 1984; Laisk & Walker 1986; Woodrow 1986; Pettersson & Ryde-Pettersson 1988; Laisk & Walker 1989; Laisk *et al.* 1989b; Gross, Kirschbaum & Pearcy 1991; Hahn 1991; Rovers & Giersch 1995; Laisk *et al.* 1997; Pearcy, Gross & He 1997; Laisk & Edwards 2000; Poolman, Fell & Thomas 2000; Laisk, Eichelmann & Oja 2006). For example, mathematical models of carbon metabolism have been developed to study the control of photosynthetic CO₂ flux within the C3 cycle in isolation (Woodrow 1986; Poolman *et al.* 2000; Poolman, Assmus & Fell 2004), photosynthetic oscillations (Laisk *et al.* 1989a; Walker 1992) or the optimization of resource use investment between the enzymes of carbon metabolism at light saturation (Zhu *et al.* 2007). Because these models were usually developed to test particular hypotheses, each model simplified processes that were not critical for testing the target hypothesis. Laisk *et al.* (2006) developed a detailed C3 photosynthesis model including both carbon metabolism and the 'light reactions', showing the growing interest in simulating the whole photosynthetic process, rather than individual parts of the system. Here we present a significantly more complete model of photosynthesis by extending these previous models, particularly the model of fluorescence induction (Zhu *et al.* 2005) and the model of carbon metabolism (Zhu *et al.* 2007). Our model presented here, *e*-photosynthesis, includes (1) the detailed reactions in the C3 cycle, sucrose synthesis, starch synthesis and photorespiration; (2) the detailed reactions associated with light absorption, excitation energy transfer, charge separation, electron transfer around both photosystem II (PSII) and photosystem I (PSI), ion transfer between the lumen and stroma, as well as ATP and NADPH synthesis; (3) the major regulatory processes involved in photosynthesis, including Rubisco activation via Rubisco activase, non-photochemical

quenching via luminal pH and the xanthophyll cycle, and the regulation of enzyme activities via the ferredoxin thioredoxin system. This article (1) describes the structure, assumptions, rate equations, differential equations and parameters used in the *e*-photosynthesis model; (2) shows that *e*-photosynthesis provides qualitatively and quantitatively realistic simulations of *in vivo* leaf photosynthesis through a series of *in silico* experiments; (3) uses *e*-photosynthesis to analyse the potential mechanisms underlying the classical chlorophyll fluorescence decay curve following induction of photosynthesis upon a dark to light transition.

MODEL DESCRIPTION

The parameters and assumptions for the reactions from water splitting to PQH₂ formation are given in Zhu *et al.* (2005) and for carbon metabolism in Zhu *et al.* (2007), and are listed in Supporting Information Appendix S1. The following explains the assumptions for the additional discrete processes added here to develop *e*-photosynthesis.

Model structure and assumptions for reactions associated with the thylakoid membrane

- 1 Reduced plastoquinone (PQH₂) is oxidized through the cytochrome b₆f complex (cyt b₆f), which consists of a c-type haem (cytochrome f), two b-type haems, an iron sulphur protein (ISP), a haem c_n (formerly known as haem X) and single molecules of chlorophyll *a* and carotenoid (Fig. 1). The mitochondrial and bacterial cyt bc₁ complex (cyt bc₁) are in the same cyt bc family as cyt b₆f and all are regarded to operate using the same modified Q cycle mechanism (Berry *et al.* 2000). Therefore, the much more prevalent kinetic parameters of reduction and oxidation in the cyt bc₁ complex were used in our model of electron transfer to describe the modified Q cycle around the cyt b₆f complex. Cyt b₆ in the cyt b₆f complex is the counterpart of cyt b in cyt bc₁; cyt f in cyt b₆f complex is the counterpart of cyt c₁ in cyt bc₁ (Berry *et al.* 2000). However, the cyt bc₁ complex lacks the chlorophyll and carotenoid molecules and cyt c_n of cyt b₆f. But since their function is unknown, they could not be included in the current version of the model.
- 2 There are three confirmed catalytic sites on cyt b₆f for binding external substrates: the plastoquinol (PQH₂) binding site (Q_p site) and the plastocyanin (PC) binding site on the lumen (p) side, and the plastoquinone (PQ) binding site on the stromal (n) side of the thylakoid membrane (Q_n site). In addition to these three catalytic sites: there are two additional catalytic interfaces (at cyt f and cyt b_{6L}), which are involved in the oxidation of PQH₂ at the Q_p site (Berry *et al.* 2000).
- 3 According to the modified Q cycle, the oxidation of PQH₂ at the Q_p site begins by formation of the substrate complex, ISP_(ox).PQH₂ (Hong *et al.* 1999; Berry *et al.* 2000; Crofts *et al.* 2000). Oxidation of ISP_(ox).PQH₂ is assumed here to occur in two steps. Firstly, one electron is

- 4 Reduced ISP coexists at equilibrium in either the protonated (ISPH) or the deprotonated state (ISP⁻) with a pK_a of 7.6 (Ugulava & Crofts 1998; Crofts *et al.* 2000). It was assumed in our model that ISPH and ISP⁻ donate electrons to cyt *f* with equal probability and are therefore represented by identical rate equations.
- 5 PQ in the Q_n site of cyt *b₆f* is assumed to become fully reduced (PQ²⁻) after receiving two electrons from the low-potential chain. The rate of protonation of PQ²⁻ has been shown to vary with pH, and the empirically derived relationship is used to capture this effect (Taly *et al.* 2003).
- 6 It is assumed that the PQH₂ formed at the Q_n site is readily available for formation of PQH₂.ISP at the Q_p site with oxidized ISP.
- 7 PSI has both core and peripheral (LHCI) antenna. Oxidized P₇₀₀ oxidizes PC, and in turn reduces a chlorophyll *a* molecule, A_0 . The other intermediate electron transfer steps between ferredoxin and A_0 are ignored (Fig. 1).
- 8 In *e*-photosynthesis, the proton motive force (pmf) for ATP synthesis incorporates both a chemical and an electrical potential across the thylakoid membrane. The observed activation behaviour of ATP synthase suggests a minimum pmf , which varies depending on the thioredoxin-regulated redox state of a pair of cysteines in the γ -subunit of ATP synthase (Ort *et al.* 1990; Ort & Oxborough 1992). It is assumed that translocation of 4.67 protons from lumen to stroma is needed for formation of 1 ATP (Vollmar *et al.* 2009).
- 9 In this model, the transport of Mg²⁺, K⁺ and Cl⁻ across the thylakoid membrane is simulated explicitly and used to calculate the electrical potential across the thylakoid membrane. The fluxes of ions between the cytoplasm and stroma are assumed not to cause significant changes in electrical potential across the thylakoid membrane (Thaler, Simonis & Schonknecht 1992). Although these ions are cofactors or effectors of some enzymes of carbon metabolism, these effects are not included in the current model, with the exception of the effect of [Mg²⁺] on Rubisco activation, as described later.
- 10 Although multiple buffer species are present in each plastid compartment, it is assumed that buffering in a compartment can be represented by a single empirical equation, which captures the observed buffering of pH (Junge *et al.* 1979; Junge & McLaughlin 1987).
- 11 *e*-Photosynthesis incorporates the regulation of light utilization through non-photochemical quenching (NPQ) following the mechanism of NPQ suggested by Crofts & Yerkes (1994). This assumes that NPQ occurs in one of the minor chlorophyll protein complexes associated with, rather than within, the reaction centre of PSII. Acidification of the lumen during illumination leads to protonation of acidic ligands (e.g. glutamine) and changes the ligating properties (Crofts & Yerkes 1994), which in turn leads to increased NPQ in the form of heat dissipation (Horton, Ruban & Walters 1996; Niyogi 1999).
- 12 It is assumed that the ratio of [PSII unit]:[cyt *b₆f*]:[PSI unit]:[PC]:[ferredoxin] = 1:1:1:1:1 and that the amount of cyt *b₆f* on a leaf area basis is 1 $\mu\text{mol m}^{-2}$, as in the model

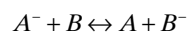
of fluorescence induction (Zhu *et al.* 2005). The volumes of the lumen and stroma were calculated from structural measurements. Specifically, a leaf is assumed to be 0.5 mm thick; 58.5% of the leaf volume is assumed to be mesophyll and 9.5% of the mesophyll cell is assumed to be chloroplast stroma (Winter, Robinson & Heldt 1994). The ratio of stroma to lumen volume varies depending on plant species, developmental stages and growth conditions (Pyke 1999). In this model, the ratio of the lumen volume to stroma volume is taken to be 1:1. Based on these assumptions, the volumes of stroma and lumen for 1 m² leaf area are $0.5 \times 10^{-3} \times 58.5\% \times 9.5\% \text{ m}^{-3} = 27 \text{ mL}$. Thus, there are 27 mL stroma and 27 mL lumen for 1 m² of leaf area.

Rate equations for reactions associated with membrane

The rate equations used in describing rate of electron transfer were derived following the assumptions and conditions described above.

The generalized rate equations

Unless stated otherwise, rate equations use generalized mass action kinetics. Where the reaction sequence is uncertain or random, the approach of convenience kinetics is used as described by Liebermeister & Klipp (2006). For electron transport, this approach is used to formulate generalized rate equations of the form A^- to B modified from Laisk & Walker (1989):



$$v = V_{\max} \left(\frac{[A^-][B]}{[A^-] + [A][B^-] + [B]} - \frac{[A][B^-]}{[A^-] + [A]([B^-] + [B])K_E} \right) \quad (1)$$

$$V_{\max} = k_{AB} \cdot \min\{[A^- + A], [B^- + B]\} \quad (2)$$

$$k_{AB} = \frac{\ln 2}{t_{1/2}} \quad (3)$$

$$\Delta E = E_B - E_A \quad (4)$$

$$\Delta G = -nF\Delta E \quad (5)$$

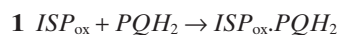
$$K_E = \exp(-\Delta G/RT) \quad (6)$$

where V_{\max} is the maximum rate of electron transport from A^- to B . k_{AB} is the rate constant of this electron transfer reaction, which was calculated from the half-time ($t_{1/2}$) of the reaction using Eqn 3 (Chang 2000). The change of the free energy of the electron transfer reaction, ΔG , was calculated based on the product of the difference between the midpoint potentials of the electron acceptor (E_B) and the electron

donor (E_A), the number of electrons transferred per molecule of product (n) and the Faraday constant (F ; Eqns 4, 5). The ΔG is further used to derive the equilibrium constant of the reaction, K_E (Eqn 6).

Rate equations for individual steps

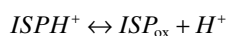
As stated in the assumptions, the reactions of cyt bc₁ (Crofts 1985; Berry *et al.* 2000) are used to represent cyt b₆f taking advantage of their functional similarity and the abundance of kinetic parameters for cyt bc₁.



$$v_{bf1} = V_{max1} \frac{[ISP_{ox}][PQH_2]}{([ISP_{ox}] + [ISPH_{(red)}])([PQ] + [PQH_2] + [PQH])} \quad (7)$$

Where V_{max1} is the maximum rate of the reaction and is assumed to be limited by the rate of PQH_2 diffusion within thylakoid membrane.

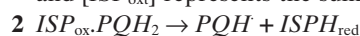
PQH_2 oxidation shows a strong pH dependency, which is due to the dependency of the deprotonation of oxidized iron-sulphur protein ($ISPH^+$) on pH (Hong *et al.* 1999). Deprotonation of $ISPH^+$ increases the amount of ISP_{ox} , and therefore, the rate of formation of $ISP_{ox} \cdot PQH_2$ (Crofts *et al.* 2000). The pK_a for $ISPH^+$ deprotonation is 7.6 for cyt bc₁ (Ugulava & Crofts 1998; Crofts *et al.* 2000). The ISP_{ox} concentration is calculated as



Since $pK = -\log \frac{[ISP_{ox}][H^+]}{[ISPH^+]}$, which can be rearranged to as

$$[ISP_{ox}] = \frac{[ISP_{ox}]_{sum}}{1 + \frac{[H^+]}{10^{-pK}}}; \quad (8)$$

where $[H^+]$ represents the luminal proton concentration and $[ISP_{ox}]_{sum}$ represents the sum of $[ISPH^+]$ and $[ISP_{ox}]$.

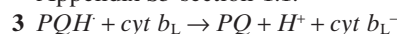


This is the first electron transfer step in PQH_2 oxidation and has a high activation barrier due to a coupled proton and electron transfer in this process (Hong & Xu 1999; Crofts *et al.* 2000). The rate equation for this reaction is assumed to be

$$v_{bf2} = k_{bf2}[ISP_{ox} \cdot PQH_2]f_{pH} \quad (9)$$

where k_{bf2} is the rate constant of this reaction and f_{pH} incorporates the effect of lumen pH on this reaction. The effect of luminal pH is incorporated by assuming that a hypothetical residue with a pK_a of 5.5 controls the rate of PQH_2 oxidation. Further, this reaction reaches its maximum rate at pH 8 and the rate then declines proportionally with the degree of protonation of the

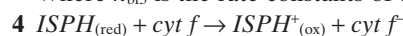
hypothetical residue with further increase in pH (Witt 1979; Nishio & Whitmarsh 1993; Cruz *et al.* 2001). The maximum rate of the electron transfer from PQH_2 to ISP_{ox} was assumed to be 150 mol s^{-1} (Crofts *et al.* 2000). The equation of f_{pH} is given in Supporting Information Appendix S3 section 1.1.



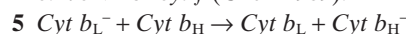
No direct measurement of the rate of this electron transfer reaction is available (Crofts *et al.* 2000). We used a value of $5 \times 10^7 \text{ s}^{-1}$ based on theoretical estimates (Hong *et al.* 1999). It is further assumed that luminal pH regulates this step in a similar manner as electron transfer from PQH_2 to ISP and this is represented by f_{pH} (Cruz *et al.* 2001). In the following six electron transfer reactions, the generalized rate constant k_{AB} of Eqn 2 is replaced by a specific rate constant for the assumed irreversible forward reaction. Since these equations determine the rate of electron transfer of the bound electron donor, this rate will be affected by the oxidation state of the acceptor, which is represented by the ratio of oxidized to total acceptor. Therefore, the rate equation for this reaction is

$$v_{bf3} = k_{bf3}f_{pH}[PQH] \frac{[Cyt b_L]}{[Cyt b_T]} \quad (10)$$

Where k_{bf3} is the rate constants of this reaction.

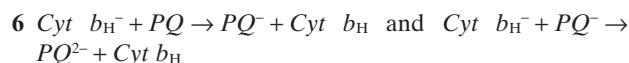


Generalized rate equations (Eqns 1–6) are used to calculate the rate of this reaction. The half-time of this reaction ($t_{1/2}$) in Eqn 3 is assumed to be 3 ms (Fernandez-Velasco *et al.* 2001). It is also assumed that the midpoint potentials (E) of Eqn 4 is 0.310 V for ISP (Hong *et al.* 1999) and 0.270 V for $cyt f$ (Chen 1989).



The maximum rate constant for the electron transfer from $cyt b_L^-$ to $cyt b_H$ is assumed to be the modal value of the theoretically calculated rate constant from QH to $cyt b_L$, that is, $5.7 \times 10^7 \text{ s}^{-1}$ (Hong *et al.* 1999; Crofts *et al.* 2000). As an approximation, we assume that b_H/b_H^- and b_L/b_L^- are isopotential, and therefore, midpoint potentials are not included in the calculation:

$$v_{bf4} = k_{bf4}[Cyt b_L^-] \frac{[Cyt b_H]}{[Cyt b_T]} \quad (11)$$



Similar to Eqns 10 and 11, the maximum rate constant for these two electron transfer steps is assumed to be $5 \times 10^7 \text{ s}^{-1}$ (Hong *et al.* 1999) and the rate equations used for these reaction are

$$v_{bf5} = k_{bf5}[Cyt b_H^-] \frac{[PQ_{nb}]}{[Cyt b_T]} \quad (12)$$

$$v_{bf6} = k_{bf6}[Cyt b_H^-] \frac{[PQ^-]}{[Cyt b_T]} \quad (13)$$

Where $[PQ_{nb}]$ represents the concentration of plastoquinone bound to the Q_n site of *cyt b₆f*. The concentration of the bound plastoquinone is calculated based on the availability of empty plastoquinone binding sites and the concentration of available free plastoquinone in thylakoid membrane. $[Q^-]$ is the concentration of unprotonated plastosemiquinone.

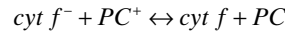
- 7** Binding of free plastoquinone (PQ) to Q_n site of *cyt b₆f*
This model assumes that the rate of PQ binding to the Q_n site depends on the concentrations of both free plastoquinone ($[PQ]$) and empty Q_n sites ($[Q_{se}]$), the rate equation for this reaction is formulated as

$$v_{bf7} = k_{bf7} [Cyt b_T] \frac{[Q_{se}] [PQ]}{[Q_{sT}] [PQ_T]} \quad (14)$$

where $[Q_{sT}]$ represents the total concentration of plastoquinone-binding sites in *cyt b₆f* and $[PQ]$ represents the concentration of free plastoquinone. $[PQ_T]$ represents the total concentration of bound and unbound plastoquinone, both oxidized and reduced. This reaction is rapid compared to PQH_2 oxidation at the Q_p site (i.e. $ISP_{ox} \cdot PQH_2 \rightarrow PQH + ISP_{red}$), which has a rate constant of 150 s^{-1} (Crofts *et al.* 2000). Therefore, as a simplification, we assumed k_{bf7} to be 10^4 s^{-1} .

- 8** Electron transfer from *cyt b₆f* to PC

As stated above (see the section *Model structure and assumptions for reactions associated with membrane*), we assume that *cyt f* and plastocyanin equal the known reactions of *cyt c₁* and *cyt c₂* of the *cyt bc₁* complex:



The general rate equations (Eqns 1–6) were used to calculate the rate of this reaction. The E_m for PC is 0.350 V and 0.270 V for *cyt f* (Chen 1989). The V_{max} for this reaction is $8.3 \times 10^6 \text{ mol L}^{-1} \text{ s}^{-1}$ (Chen 1989).

- 9** Electron transfer from plastocyanin to P_{700}

The rate equation for this reaction is assumed as

$$v_{bf10} = k_{bf10} \left(\frac{[PC][P_{700}^+]}{[P_{700T}]} - \frac{[PC^+][P_{700}]}{[P_{700T}]K_{10}} \right) \quad (15)$$

where $[P_{700T}]$ represents the total concentration of P_{700} and the k_{bf10} is calculated based on a $t_{1/2}$ of $4 \mu\text{s}$ (Bowyer, Tierney & Crofts 1979a,b) and K_{10} is the equilibrium constant of this reaction.

- 10** Plastoquinone protonation

Formation of PQH_2 from PQ^{2-} was assumed to occur with a V_{max} as $5.7 \times 10^7 \text{ s}^{-1}$, based on the theoretical calculation of the rate of electron transfer from PQH to *cyt b_L* (Hong *et al.* 1999). The concentration of the reduced plastoquinol at the Q_n site ($[PQ^{2-}]$) and the stromal pH influence the rate of plastoquinone protonation. This is represented as

$$v_{qi} = 2k_{qi} [PQ^{2-}] f_{ph2} \quad (16)$$

where k_{qi} is the rate constant for this reaction, f_{ph2} incorporates the effects of pH on this reaction, which is derived

from empirical data for the protonation of PQ_B^{2-} (Taly *et al.* 2003), which we assume to behave similarly to PQ^{2-} bound at the Q_n site.

- 11** ATP synthesis

The rate of ATP synthesis was assumed to follow Michaelis–Menten kinetics (Eqn 17). The equilibrium constant for ATP synthesis is calculated based on the Gibbs free energy of the reaction (Eqn 18), which is in turn determined by the proton motive force including both $\Delta\Psi$ and ΔpH components and the standard Gibbs free energy for this reaction (ΔG°). $\Delta\Psi$ is calculated using Eqn 22 described later. The contribution of ΔpH to the Gibbs free energy is represented by $0.592 HPR (\ln[H_n]/[H_{is}])$ where HPR is the proton/ ATP ratio, that is, the number of proton translocation needed for formation of 1 ATP . In this model, HPR is assumed to be 4.67 (Vollmar *et al.* 2009).

$$v_{bf11} = \frac{V_{bf11max} \left([ADP][Pi] - \frac{[ATP]}{kE} \right)}{(K_{mADP}K_{mP}) \left(1 + \frac{[ADP]}{K_{mADP}} + \frac{[Pi]}{K_{mP}} + \frac{[ATP]}{K_{mATP}} + \frac{[ADP][Pi]}{K_{mADP}K_{mP}} \right)} \quad (17)$$

$$kE = e^{(-\Delta G/RT)} \quad (18)$$

$$\Delta G = \Delta G^\circ + 0.592 HPR \ln \left(\frac{[H_n]}{[H_{is}]} \right) + HPR \Delta\Psi \quad (19)$$

where $V_{bf11max}$ is the maximum rate of this reaction; H_n and H_{is} represent the concentrations of proton in the lumen and stroma, respectively, which were calculated using standard buffering equations (Eqns 24, 25). K_{mADP} , K_{mATP} , K_{mP} represent the Michaelis–Menten constants for ADP, ATP and Pi.

- 12** Ion movement through the thylakoid membrane

In order to calculate $\Delta\Psi$, the movements of ions across thylakoid membrane must be simulated. These are driven by transmembrane electrical and concentration differences, which is described by the Nernst–Planck equation (Eqn 20). Equation 21 is the solution of this equation used in *e*-photosynthesis to calculate ion flux (Bockris & Reddy 1970). Here, the fluxes of ions across the thylakoid membrane depend on $\Delta\Psi$, the luminal concentration of the ion (I_i), the stromal concentration of the ion (I_s) and the permeability constant (P) for the ion. The fluxes of K^+ , Mg^{2+} and Cl^- were calculated individually with this equation. The electrical potential across the thylakoid membrane, $\Delta\Psi$, was calculated based on the difference in charges between the stroma (Q_c) and lumen and electrical capacitance (C) of the thylakoid membrane (Eqns 22 and 23). The net charge in the thylakoid lumen is equal and opposite to that in the stroma; therefore, the difference in charge between stroma and lumen is equal to twice the net charge in stroma (Eqn 22). The ratio of stroma volume per unit thylakoid membrane area follows (Flores, Graan & Ort 1983; Cruz *et al.* 2001). As a

simplification, we assumed that the net charge in stroma and lumen is zero for dark-adapted leaves; therefore, the net charge across thylakoid membrane as a result of ion transfer and proton translocation is equal to twice the net charge in the stroma or in the lumen (Eqns 22 and 23).

$$J = -\mu RT \frac{d[I]}{dx} - zF\mu \frac{d\Psi}{dx} \quad (20)$$

$$J = P \frac{zF\Delta\Psi}{RT} \frac{([I_i] - [I_e] e^{-\frac{zF\Delta\Psi}{RT}})}{1 - e^{-\frac{zF\Delta\Psi}{RT}}} \quad (21)$$

$$\Delta\Psi = \frac{2Q_c}{C} \quad (22)$$

$$Q_c = F([K_s^+] + [H_s^+] + 2[Mg_s^{2+}] - [Cl_s^-] - [OH_s^-] - [BF_s^-]) \quad (23)$$

where, $[OH_s^-]$ and $[BF_s^-]$ are the concentrations of hydroxyl ions and the buffer species, respectively, in the stroma (s). Chloroplast $[Mg^{2+}]$ ranges from 2 to 18 mM, a significant amount of which is possibly bound to thylakoid membrane, LHC complexes and nucleotides (Barber 1976; Schropelmeier & Kaiser 1988). K^+ and Na^+ are also major cations in the chloroplast (Schropelmeier & Kaiser 1988). The permeability of Mg^{2+} and K^+ through thylakoid cation channels is similar (Pottosin & Schonknecht 1996). No report on the permeability to Na^{2+} is available currently. K^+ and Mg^{2+} are assumed to be the major cations, which can permeate through the thylakoid membrane and therefore are the only ones included in this model.

Cl^- was assumed in our model to be the only anion, which can permeate through the thylakoid membrane between the stroma and lumen. The cytoplasmic $[Cl^-]$ has been estimated to be 1 to 3 mM (Schropelmeier & Kaiser 1988; Thaler *et al.* 1992). The permeability coefficient of Cl^- is assumed as $1.8 \times 10^{-8} \text{ cm s}^{-1}$ as used by Cruz *et al.* (2001). As a simplification, it was assumed that in a dark-adapted leaf, the resting membrane potential is zero and that the different ions have equal concentrations in the stroma and the lumen.

The membrane electrical capacitance (C in Eqn 22) is approximately $0.6\text{--}1 \mu\text{F cm}^{-2}$ (Vredenberg 1976; Junge *et al.* 1979) and the ratio of lumen volume to thylakoid membrane single surface area was assumed to be 0.8 nL cm^{-2} (Vredenberg 1976; Vredenberg & Bulychev 1976).

13 Calculation of pH in stroma and lumen

Four photosynthetic reactions influence the combined total concentration of protons and protonated buffer species in lumen ($[H^+] + [BFH]$), that is, water oxidation ($v_{s3,so}$ in appendix 2 of Zhu *et al.* 2005), the electron transfer from PQH⁺ to cyt b_L (Eqn 10), electron transfer from ISPH⁺ to cyt f (v_{b8} in section 1.1 of Supporting Information Appendix S1) and ATP synthesis (Eqn 17). Four related photosynthetic reactions influence ($[H^+] + [BFH]$) in the stroma, that is, ATP synthesis (Eqn 17), proton uptake at the Q_n site of cytb₆f complex (Eqn 16), proton

uptake at the Q_B site of PSII (v_{qb} in section 1.1 of Supporting Information Appendix S1) and NADPH formation (Eqn 33a).

Considering that several distinct buffer species exist in the stroma and the lumen, the pH of the stroma and lumen were calculated based on the measured buffer capacities and the changes in $[H^+ + BFH]$ for each compartment. The buffer capacity for a group of buffer species is derived from the equilibrium equation for each individual buffer species. For example, for the i th buffer species in this group, the equilibrium equation is

$$K_i = \frac{[H^+][BF_i^-]}{[BF_iH]} \quad (24)$$

where K_i is the dissociation constant for proton binding to buffering group BF_i^- ; $[BF_i^-]$ and $[BF_iH]$ are the concentrations of the deprotonated and protonated i th buffer species. The range of pKa values of the many buffering groups results in a linear change in pH in proportion to translocation of protons (Junge *et al.* 1979; Junge & McLaughlin 1987). The buffering capacity (K_b) is therefore defined as

$$K_b = \frac{\Delta([H^+] + \sum_{i=1}^n [B_iH])}{\Delta(\text{pH})} \quad (25)$$

In this model, the buffer capacities for lumen and stroma were assumed to be 0.03 and $0.02 \text{ mol L}^{-1} (\text{pH unit})^{-1}$, respectively (Oja *et al.* 1999; Cruz *et al.* 2001).

14 Excitation energy absorption and transfer, and electron transport reactions around PSI

The excited states of chlorophylls in the two antenna systems (peripheral antenna A_{IP} and core antenna U_1 , Fig. 1) have one of three fates: photochemistry, heat dissipation and fluorescence with rate equations as follows:

$$v_{IPC} = [A_{IP}]k_{AU} \quad (26)$$

$$v_{ICP} = [U_1]k_{UA} \quad (27)$$

$$v_f = ([A_{IP}] + [U_1])k_{f,ps1} \quad (28)$$

$$v_d = ([A_{IP}] + [U_1])k_d \quad (29)$$

where v_{IPC} represents the rate of excitation energy transfer from the peripheral antenna to the core antenna of PSI; v_{ICP} represents the rate of excitation energy transfer from the core antenna to the peripheral antenna of PSI; v_f represents the rate of fluorescence emission from antenna, which is essentially zero for PS1 due to P700 quenching. Therefore, $k_{f,ps1}$ is assumed to be zero. Finally, v_d represents the rate of heat dissipation from the antenna and k_{AU} and k_{UA} represent the rate constants of excitation transfer from A_{IP} to U_1 , and from U_1 to A_{IP} , respectively.

15 Primary charge separation at the PSI reaction centre

$P_{700e} + A_0 \leftrightarrow P_{700e}^+ + A_0$ where P_{700e} represents the excited PSI reaction centre (P_{700}). As previously assumed for P_{680} , P_{700} is assumed always to be in equilibrium with the excited chlorophylls in the core antenna. The proportion of excited P_{700} chlorophylls is given as

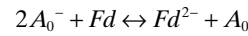
$$[P_{700e}] = [U_1] \frac{([P_{700T}] - [P_{700}^+])}{120} \quad (30)$$

where 120 represents the number of chlorophylls in the core antenna of PSI including P_{700} (Horton *et al.* 1996; Chitnis 2001).

The rate of primary charge separation in PSI is assumed to be

$$v_{bf15} = k_{15} [P_{700e}] \frac{[A_0]}{[A_{0T}]} \quad (31)$$

where $[A_0]/[A_{0T}]$ is the proportion of open primary acceptors of PSI, k_{15} is the rate constant for PSI primary charge separation, which was calculated based on a half-time ($t_{1/2}$) of 30 ps (Chitnis 2001).

16 Electron transport from A_0^- to ferredoxin

The half-time ($t_{1/2}$) for electron transfer from A_0 to ferredoxin was assumed to be 200 ns and this is incorporated into k_{16} below (Chitnis 2001). The rate equation for this reaction is

$$v_{bf16} = k_{16} [A_0^-] \frac{[Fd]}{[Fd_T]} \quad (32)$$

where $[Fd_T]$ is the total concentration of ferredoxin ($[Fd_T] = [Fd] + [Fd_r]$) where $[Fd]$ and $[Fd_r]$ are the concentrations of oxidized and reduced ferredoxin, respectively.

17 The formation of NADPH

The detailed kinetics of the electron transfer process between Fd_r and $NADP^+$ are not known. Fd has been suggested to form a rigid complex with ferredoxin-NADP reductase (FNR) (Laisk *et al.* 1992; Laisk 1993; Lelong *et al.* 1994). Since electron transfer reactions are usually very fast in this complex, as a simplification, in *e*-photosynthesis, it is assumed that availability of $NADP^+$ is the limiting step for generation of NADPH. A simple one-substrate one-product Michaelis–Menten rate equation is therefore used to describe this reaction, as in Fridlyand *et al.* (1999):

$$v_{bfm2} = \frac{V_{2M} \left(\frac{[Fd_r]}{[Fd_T]} [NADP^+] - \frac{[Fd]}{[Fd_r]} \frac{[NADPH]}{K_2} \right)}{K_{mNADP} \left(1 + \frac{[NADP^+]}{K_{mNADP}} + \frac{[NADPH]}{K_{mNADPH}} \right)} \quad (33a)$$

where v_{bfm2} is the rate of this reaction, K_{mNADP} and K_{mNADPH} are the Michaelis–Menten constants for *NADP*

and *NADPH*, respectively, V_{2M} is the maximum rate of the forward reaction, K_2 is the equilibrium constant for this reaction, which is determined by the difference in redox potential between Fd/Fd_r (about -0.420 V) and $NADP/NADPH$ (about -0.340 V) at pH 8 (Keirns & Wang 1972; Knaff 1996). Following Fridlyand *et al.* (1999), the maximum rate of electron transfer from Fd_r to *NADP* is $1600 e^- s^{-1}$, which corresponds to a maximum rate of *NADPH* generation of $27.8 \text{ mmol L}^{-1} s^{-1}$ based on the assumed ferredoxin concentration and standard dimensions of leaf and chloroplasts used in the model.

18 Cyclic electron transfer

In *e*-photosynthesis, we assume that the cyclic electron transfer is continuously engaged (Joliot & Joliot 2002). Though there are various proposed mechanisms of cyclic electron transfer (Bendall & Manasse 1995; Shikanai 2007). Here we assume the simplest and widely accepted model that the electron transfer to the plastoquinone bound to the Q_n site is rate dependent on the redox state of the ferredoxin and concentration of plastoquinone bound to the Q_n site $[PQ_n]$:

$$v_{cet} = V_{cetm} [PQ_n] [Fd_r] / [Fd_T] \quad (33b)$$

where V_{cetm} is the maximal rate of cyclic electron transfer. By setting V_{cetm} to zero, the model will simulate a photosynthetic apparatus with no cyclic electron transfer.

Rate equations associated with regulatory mechanisms*Reactions associated with NPQ*

The mechanism of NPQ proposed by Crofts & Yerkes (1994) is incorporated into the model (See the section, *Model structure and assumptions used in the model*). In summary, this assumes that decrease in luminal pH increases the protonation of a putative ligand (q_{H^+}) causing a conformational change in the quenching site in turn increasing the rate constant for of heat dissipation (k_d). The pK_a value of the putative ligand is assumed to be 4.5 (Gilmore 1997). A differential equation describing the rate of change in k_d (Laisk *et al.* 1997) is used:

$$\frac{dk_d}{dt} = k_r (q_{H^+} \cdot k_{dm} - k_d) \quad (34)$$

where:

$$q_{H^+} = \frac{[H_{fl}]}{[H_{fl}] + K_E} \quad (35)$$

$$K_E = 10^{-pK} \quad (36)$$

where $[H_{fl}]$ is the proton concentration in lumen, k_{dm} is the maximum rate constant for heat dissipation and k_r describes the rate of relaxation of the rate constant of heat dissipation.

Activation of Rubisco by Rubisco activase

The order of substrate binding is critical for normal functioning of Rubisco. Rubisco is carbamylated by forming a complex with CO₂ and Mg²⁺. Carbamylated Rubisco can bind RuBP and in turn CO₂ or O₂ leading to carboxylation or oxygenation (Fig. 1b). If, however, Rubisco binds RuBP before binding CO₂ and Mg²⁺ (uncarbamylated), is assumed to be inactive. Rubisco activase increases the rate constant for the release of RuBP minimizing this inactivation (Portis 1995, Portis, 2003). These processes were explicitly incorporated into *e*-photosynthesis. The detailed equations describing the reactions involved in Rubisco activation and deactivation (Fig. 1b) are given in Supporting Information Appendix S3 section 1.1. The key assumptions are described here. Following Mott & Woodrow (2000), the rate constant for activating Rubisco (k_{ra}) is

$$k_{ra} = \frac{[\text{activase}]}{13014} \quad (37)$$

where [activase] represents the concentrations of Rubisco activase for which 13014 s mg [activase] m⁻² is an empirically derived constant (Mott & Woodrow 2000).

The activity of Rubisco activase is assumed to be regulated by the ratio of stromal ADP to ATP concentrations, following Zhang & Portis (1999).

The rate of RuBP dissociation from Rubisco (v_{ra1}) is calculated as

$$v_{ra1} = k_{ra}[ER] \cdot \max\{(1 - [ADP]/(3[ATP])), 0\} \quad (38)$$

where [ER] is the concentration of RuBP bound to Rubisco.

The rate of formation of [ER] (v_{ran1}) is assumed to follow mass action:

$$v_{ran1} = k_{n1}[E][RuBP] \quad (39)$$

where k_{n1} is based on the reported time needed for Rubisco inactivation (Ernstsen, Woodrow & Mott 1999).

In the model, [E], [EC] and [ECM] remain in equilibrium (Fig 1b) using the equilibrium constants of Mate *et al.* (1996). The rate of formation of ECMR, that is, carbamylated Rubisco with bound RuBP and Mg²⁺, is calculated as

$$v_{ra7} = k_{ra7}[ECM][RuBP] \quad (40)$$

There are no measurements for this rate constant but since it is assumed not to be rate limiting, k_{ra7} was set to 10 times the catalytic number for carboxylation by active sites of Rubisco, giving 25 s⁻¹.

The rate of RuBP dissociation from ECMR has been found to be very slow compared to the rate of catalytic conversion of ECMR to PGA (Portis 1995), this observation was approximated in the model by assuming a dissociation constant (k_{ran7}) of 0.5 s⁻¹:

$$v_{ran7} = k_{ran7}[ECMR] \quad (41)$$

The xanthophyll cycle

The xanthophyll cycle, which involves interconversion among zeaxanthin (Zx), antheroxanthin (Ax) and violaxanthin (Vx), is critical for photoprotection of the photosynthetic apparatus by the thermal dissipation of absorbed energy. It is assumed that the interconversions among Vx, Ax and Zx follow first-order kinetics (Eqns 42–45). The initial concentrations of Vx, Ax and Zx as well as the rate constants for conversions of Vx to Ax and of Ax to Zx were from experimentally determined values (Frommolt, Goss & Wilhelm 2001; Table 2.4 in Supporting Information Appendix S2). The influence of changes in luminal pH on the rate constants of conversion from Vx to Ax, and from Ax to Zx was described by assuming the rate constants of Vx to Ax, and from Ax to Zx are at their maximum when luminal pH is lower than 5.2 (Frommolt *et al.* 2001) and that these two rate constants decrease linearly when luminal pH is higher than 5.2 reaching zero at pH ≥ 6.5 (Supporting Information Appendix S3; section 1.1). X_{state} , defined as $[Zx]/([Ax] + [Vx] + [Zx])$, was used to predict the maximum rate constant of heat dissipation (d_m). The maximal rate ‘constant’ for heat dissipation (k_{dm}) is inversely related to X_{state} (Eqns 34–36, 48). The sum of [Ax], [Vx] and [Zx] is assumed constant throughout. Although referred to as a rate constant (k_d), this apparent rate constant will vary. Here we assume this variation may be described via dynamics of zeaxanthin concentration and luminal pH. Demmig-Adams & Adams (1996) quantified the impacts of xanthophyll cycle components on heat dissipation rate constant. As an approximation, this model assumes a minimum k_{dm} at $X_{state} \leq 0.3$, defined by k_{d0} . At $X_{state} > 0.3$, k_{dm} is increased as a function of X_{state} , divided by 0.3 so that k_{dm} will never be less than k_{dm0} and will be increased by about 3.3 times when X_{state} becomes 1 (Eqn 48). Change in the k_r is similarly calculated (Eqn 49). These values of k_r and k_{dm} are then substituted into Eqn 34 to simulate the dual effects of X_{state} and pH on k_d .

$$v_{av} = [Ax]k_{av} \quad (42)$$

$$v_{va} = [Vx]k_{va}pHReg \quad (43)$$

$$v_{az} = [Ax]k_{az}pHReg \quad (44)$$

$$v_{za} = [Zx]k_{za} \quad (45)$$

$$pHReg = 1 \quad (pH_l \leq 5.8)$$

$$pHReg = \frac{6.5 - pH_l}{0.7} \quad (6.5 > pH_l > 5.8) \quad (46)$$

$$pHReg = 0 \quad (pH_l > 6.5)$$

$$X_{state} = \frac{[Zx]}{[Ax] + [Vx] + [Zx]} \quad (47)$$

$$k_{dm} = k_{dm0} \max\{X_{state}/0.3, 1\} \quad (48)$$

$$k_r = k_{r0} \max\{X_{\text{state}}/0.3, 1\} \quad (49)$$

Regulation of enzyme activity via thioredoxin

e-Photosynthesis incorporates thioredoxin regulation of sedoheptulose-1:7-bisphosphatase (SBPase), fructose-1:6-bisphosphatase (FBPase), phosphoribulose kinase (PRK), glyceraldehyde-3-phosphate dehydrogenase (GAPDH), ADP-glucose pyrophosphorylase (ADPGPP), rubisco activase (activase) and ATP synthase (ATPase). Thioredoxin regulates the activities of these enzymes by thiol/disulfide exchange, reducing disulfide (-s-s-) on the inactive form of an enzyme to sulfhydryl (-SH) groups yielding the active enzyme and vice-versa (Schurmann & Buchanan 2001). A standard rate equation describing electron transfer reactions between two redox components was used to describe the electron transfer between enzymes and thioredoxin (Laisk & Walker 1989; Chang 2000). For example, the electron transfer rate from thioredoxin to phosphoribulose kinase (PRK) ($v_{e2\text{PRK}}$) is calculated as:

$$v_{e2\text{PRK}} = k_{e2\text{PRK}} \left([\text{Thio}_r][\text{PRK}_o] - \frac{[\text{Thio}_o][\text{PRK}_r]}{KE_{2\text{PRK}}} \right) \quad (50)$$

where $k_{e2\text{PRK}}$ is the rate constant of electron transfer from reduced thioredoxin (Thio_r) to oxidized PRK (PRK_o). $[\text{PRK}_r]$ and $[\text{Thio}_o]$ represent the concentrations of reduced PRK and oxidized thioredoxin, respectively. $KE_{2\text{PRK}}$ represents the equilibrium constant of the electron transfer between thioredoxin and PRK, which was estimated based on the difference between midpoint potentials of thioredoxin and PRK (Eqn 6). The redox potentials and concentrations of these different enzymes, rate constants of electron transfer from thioredoxin to these different enzymes were obtained from literature (Supporting Information Appendix S2, Table 2.2) Thioredoxin was reduced subsequently by ferredoxin via ferredoxin-thioredoxin reductase (Supporting Information Appendix S3, section 1.1).

MODEL REPRESENTATION AND ALGORITHMS

e-Photosynthesis, combines all reactions in the model of carbon metabolism (Zhu *et al.* 2007), the model of fluorescence induction (Zhu *et al.* 2005), as well as the electron transfer reactions around cyt *b*₆f and PSI, ATP and NADPH generation, as well as the regulatory mechanisms described above. The procedure used in building the model of carbon metabolism and fluorescence induction (Zhu *et al.* 2005, 2007; Zhu 2010) was used here to achieve *e*-photosynthesis. The system of ordinary differential equations representing the structure of *e*-photosynthesis was solved numerically using *ode15s* of MATLAB (v6, the Mathworks, Inc, Natick, MA, USA). The structural and kinetic properties of enzymes/components used in *e*-photosynthesis were collected from the peer reviewed literature (Supporting Information Appendix S2, Tables 2.1 to 2.3).

NUMERICAL EXPERIMENTS

The initial concentrations of components in photosynthesis were based on those in a representative sunlit leaf of an herbaceous C3 dicot (see Zhu *et al.* 2005; Zhu *et al.* 2007; Supporting Information Appendix S2, Tables 2.4 and 2.5).

Experiment 1

An *in silico* perturbation experiment was conducted to investigate the ability of *e*-photosynthesis to attain a steady state and reliably regain that steady state after a simulated environmental perturbation. Specifically, in the model, steady state was attained at a photosynthetically active photon flux density (PFD) of 1000 $\mu\text{mol m}^{-2} \text{s}^{-1}$. Then after 200 s, PFD was decreased to 100 $\mu\text{mol m}^{-2} \text{s}^{-1}$ for 200 s, and then returned to 1000 $\mu\text{mol m}^{-2} \text{s}^{-1}$.

Experiment 2

To assess the criticality of specific model parameters, a sensitivity analysis was conducted. Parameters were individually decreased by 20% and 80%, under low and high light, and under current and elevated atmospheric $[\text{CO}_2]$.

Experiment 3

e-Photosynthesis was tested for its ability to reproduce typical responses of leaf CO_2 uptake to intercellular CO_2 concentration (A/c_i curve) and to PFD (A/PFD curve). These were obtained by working stepwise through a range of c_i and of PFD, allowing a steady-state A to be achieved at each step.

Experiment 4

e-Photosynthesis was examined for its ability to mimic modulated chlorophyll fluorescence quenching. A typical *in vivo* quenching analysis protocol was used as described in the legend of Fig. 6.

RESULTS

Experiment 1

Despite rate constants in the system of differential equations spanning 11 orders of magnitude, the system successfully attained a steady state, regained a new steady state following a 10-fold decrease in PFD, and then successfully returned to the original steady state when returned to the original PFD (Fig. 2). Further, *e*-photosynthesis gave quantitatively and temporally realistic predictions of the dynamics of CO_2 uptake (A), O_2 evolution, heat dissipation and the quantum yield of PSII (Φ_{PSII}), chlorophyll fluorescence, membrane potential, lumenal and stromal pH (Fig. 2). For example, the predicted A of 15 and 5 $\mu\text{mol m}^{-2} \text{s}^{-1}$ at 1000 and 100 $\mu\text{mol m}^{-2} \text{s}^{-1}$ under current CO_2 and O_2 levels are within the range of commonly measured A for a healthy C3 leaf (Wullschlegel 1993). Furthermore, the increase in the

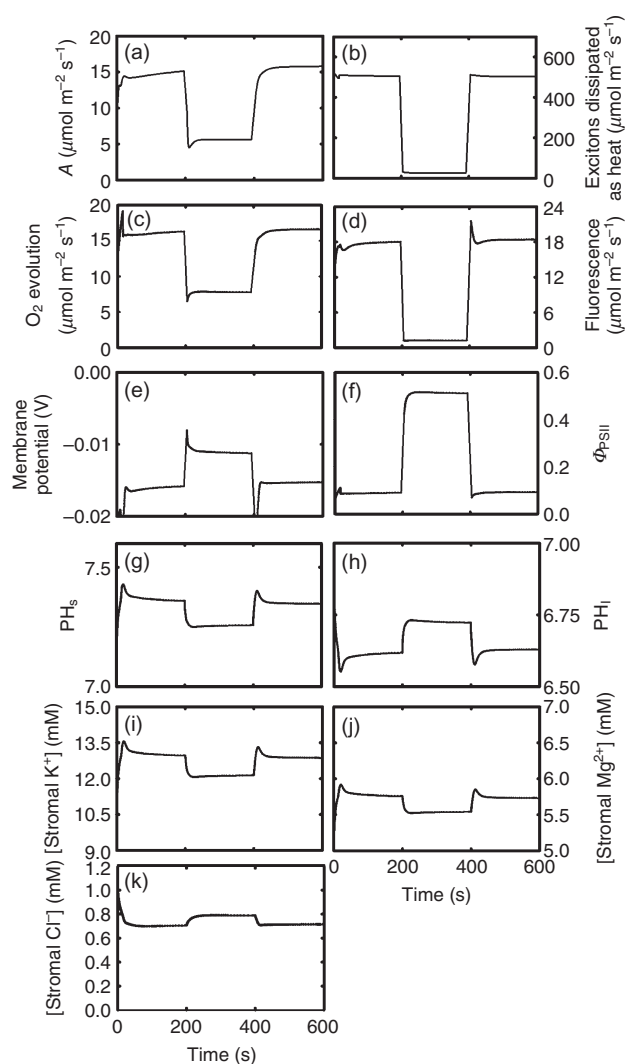


Figure 2. Predicted responses of photosynthesis and chloroplast properties in response to a 10-fold reduction in photon flux density (PFD) and return to the original PFD. The structural and kinetic properties of enzymes or components used in *e*-photosynthesis (Tables 2.2 and 2.3 in Supporting Information Appendix S2) are based on literature for a 'typical' terrestrial C3 leaf, as described previously Zhu *et al.* (2005, 2007). The initial concentrations of different intermediates and parameters are given in Tables 2.4 and 2.5 of Supporting Information Appendix S2. Intercellular CO₂ and O₂ concentrations were set to be 280 μmol mol⁻¹ and 210 mmol mol⁻¹, respectively. Temperature was 25 °C and PFD 1000 μmol m⁻² s⁻¹ for 0–200 s, 100 μmol m⁻² s⁻¹ for 200–400 s, returning to 1000 μmol m⁻² s⁻¹. (a) Net leaf photosynthetic CO₂ uptake rate (*A*); (b) 'excitons' dissipated as heat; (c) the rate of O₂ evolution by photosystem II (PSII); (d) chlorophyll fluorescence; (e) membrane potential; (f) quantum yield of PSII; (g) stromal pH; (h) lumenal pH; (i) stromal [K⁺]; (j) stromal [Mg²⁺]; and (k) stromal [Cl⁻].

proportion of excitation energy dissipated as heat (Fig. 2b) and a decrease in quantum yield of PSII under high light (Fig. 2f) are consistent with vast amount of experimental observations as well; see reviews in (Long, Humphries & Falkowski 1994; Horton *et al.* 1996; Ort 2001).

Experiment 2

Sensitivity analysis: unsurprisingly, the predicted steady state rate of net CO₂ uptake (*A*) was very sensitive to the assumed number of protons required to produce one ATP (Table 1). At high [CO₂] and PFD, assuming 4 in place of 4.67 increased *A* by 22%. At low light, decreasing other parameters by 20% had little effect on the predicted *A*; however, decreasing ATP/H⁺ had a very significant effect (Table 1). This is consistent with expectation since under light-limiting conditions, the efficiency of energy transduction into NADPH and ATP will be critical to the overall rate of photosynthesis. Of the 11 further parameters tested, only a 20% decrease in the concentrations of FBPase, SBPase, Cyt b₆f and Rubisco caused a decrease in *A* in high light (Table 1). At elevated [CO₂] similar decreases were observed excepting that *A* became insensitive to a 20% decrease in Rubisco, which is consistent with the fact that this enzyme is more efficient as [CO₂] is increased (e.g. Long *et al.*, 2004). When decreased by 80%, FBPase, SBPase, Rubisco, Cyt b₆f and ATP synthase caused c. 40–75% reductions in *A*, in high light and at both levels of [CO₂]. The rate of formation of carbamylated Rubisco (ECM) with RubP is determined by the rate constant *k*_{ra7}. No clear value of this critical rate constant was available. This analysis showed that *k*_{ra7} inserts little control over photosynthetic CO₂ uptake under both current and future elevated [CO₂] (Table 1).

Experiment 3 and 4

In a simulated experiment, leaf photosynthesis was allowed to achieve steady state at a PFD of 1000 μmol m⁻² s⁻¹, and then PFD was decreased by a step of 100 μmol m⁻² s⁻¹ every 200 s, achieving a new steady-state, before each decrease. Changes in all parameters and quantitative values, for example, the CO₂ uptake rate and oxygen evolution rate, generally reflect those typically seen in conducting such experiments in healthy C3 leaves (Fig. 3; von Caemmerer 2000). When the data are used to reconstruct the response of *A* to PFD, a typical response curve may be seen with an initial linear response to PFD in low light and saturation at about 500 μmol m⁻² s⁻¹ (Fig. 3j). Similarly, an experiment in which the response of *A* in saturating light to intercellular [CO₂] was simulated by running photosynthesis to steady state at a *c*_i of 1000 μmol mol⁻¹ and then decreasing *c*_i in steps of 100 μmol mol⁻¹ at 200 s intervals, allowing steady state to be achieved in each step (Fig. 4). Again, the response pattern and quantitative value of key measures are consistent with those observed *in vivo*. When the data are used to reconstruct the response of *A* to *c*_i, a typical response curve of a light-adapted C3 leaf may be seen with a high *dA/dc*_i at low *c*_i where photosynthesis is RuBP saturated and declining to near saturation at a *c*_i above c. 300 μmol mol⁻¹ (Fig. 4j).

Experiment 5

Leaf photosynthesis was allowed to reach steady state at a PFD of 2000 μmol m⁻² s⁻¹ and *c*_i of 280 μmol mol⁻¹, and

| | | [CO ₂] (μmol mol ⁻¹) | | | |
|---------------------|---|--|-------|-------|-------|
| | | 280 | 560 | | |
| Scaling coefficient | PFD (μmol m ⁻² s ⁻¹) | 200 | 2000 | 200 | 2000 |
| 1 | Control | 8.34 | 15.9 | 10.6 | 20.82 |
| HPR = 4 | HPR | 8.91 | 17.3 | 11.31 | 25 |
| Decrease by 20% | [FBPase] | 8.32 | 15.5 | 10.6 | 20.26 |
| | [SBPase] | 8.3 | 15.8 | 10.6 | 20.67 |
| | [Cyt b ₆ f] | 8.34 | 15.2 | 10.6 | 19.88 |
| | [Fd _r] | 8.34 | 15.9 | 10.6 | 20.8 |
| | [P _{700r}] | 8.34 | 15.9 | 10.6 | 20.8 |
| | [ATP synthase] | 8.3 | 15.9 | 10.6 | 20.8 |
| | [PSII centre] | 8.34 | 15.9 | 10.6 | 20.8 |
| | [activase] | 8.34 | 15.9 | 10.6 | 20.8 |
| | [OEC] | 8.34 | 15.9 | 10.6 | 20.8 |
| | kra7 | 8.34 | 15.9 | 10.6 | 20.8 |
| Decrease by 80% | [Rubisco] | 8.4 | 14.46 | 10.68 | 20.8 |
| | [FBPase] | 4.16 | 4.46 | 5.25 | 5.34 |
| | [SBPase] | 7.33 | 9.72 | 9.36 | 12.47 |
| | [Cyt b ₆ f] | 7.05 | 6.99 | 8.96 | 9.17 |
| | [Fd _r] | 8.34 | 15.9 | 10.61 | 20.82 |
| | [P _{700r}] | 8.34 | 15.9 | 10.61 | 20.82 |
| | [ATP synthase] | 6.74 | 6.89 | 8.55 | 8.6 |
| | [PSII centre] | 8.34 | 15.9 | 10.61 | 20.82 |
| | [activase] | 8.34 | 15.9 | 10.61 | 20.82 |
| | [OEC] | 8.34 | 15.9 | 10.61 | 20.82 |
| kra7 | 8.34 | 15.9 | 10.7 | 20.8 | |
| [Rubisco] | 3.7 | 3.79 | 6.52 | 6.61 | |

Table 1. Sensitivity analysis of chosen parameters in *e*-photosynthesis on photosynthetic CO₂ uptake rate (μmol m⁻² s⁻¹)

The photosynthetic CO₂ uptake rate is calculated as the rate of RuBP carboxylation minus the rate of CO₂ release by glycine decarboxylase. The sensitivity analysis was conducted by decreasing the default parameter values by either 20% or by 80%. The sensitivity analysis was conducted for intercellular CO₂ concentrations corresponding to current (280 μmol mol⁻¹) and elevated CO₂ concentrations (560 μmol mol⁻¹) under low (200 μmol m⁻² s⁻¹) and high (2000 μmol m⁻² s⁻¹) PFDs.

returned to darkness. After a brief period, the leaf was returned to a PFD of 2000 μmol m⁻² s⁻¹ and induction and quenching of chlorophyll fluorescence was tracked and analysed with simulated saturating light flashes. Figure 5 shows the initial fluorescence transient and Fig. 6 analyses this further with a series of saturating flashes. Fluorescence transients show the typical OPMST series of transients in emission (Fig. 5). On dark-light transition, a burst of O₂ release is indicated and a prompt rise in fluorescence followed by quenching, coupled with a rise in NPQ (Fig. 6) mimicking typically observed changes in leaf chlorophyll fluorescence *in vivo*.

DISCUSSION

The induction of photosynthesis following a dark to light transition was realistically simulated showing a gradual increase in *A* upon illumination (Fig. 2a), which was the result of gradual activation of different enzymes involved in the C3 cycle, that is, SBPase, PRK, GAPDH, ADPGPP and Rubisco activase by the ferredoxin-thioredoxin system (Schurmann & Jacquot 2000). One caveat is that induction of *A* was complete within about 200 s. In an intact leaf, complete induction typically requires more time; however, this is likely due to the slower opening of the stomata. The current version of *e*-photosynthesis does not include stomatal dynamics or

any diffusive limitation to CO₂ access to the stroma. However, this length of induction is consistent with rates observed in isolated protoplasts of wheat mesophyll cells, which would not be affected by stomatal and other diffusive limitations. Here, steady state was achieved within 240 s of a dark-light transition (Leegood & Walker 1981).

Oscillations in CO₂ uptake and O₂ evolution, which have often been observed in leaves following rapid changes in light and CO₂ levels (Walker 1992), were predicted by *e*-photosynthesis when PFD was abruptly changed (Fig. 2a,c). At a low light level (100 μmol m⁻² s⁻¹), the resting membrane potential is about -11 mV; decreasing to about -15 mV under high light level (1000 μmol m⁻² s⁻¹) after 200 s (Figs 2e & 3e). This change in the trans-membrane electrical potential was caused by changes in the concentration of charged ions (Mg²⁺, K⁺, Cl⁻, H⁺, OH⁻) between the lumen and stroma. More specifically, the change in trans-membrane potential under high light is caused by an increase in luminal [H⁺] counteracted by decreases in concentrations of luminal Mg²⁺, K⁺ and increase in concentration of luminal Cl⁻ (Fig. 2i,j,k). These changes are consistent with observed ion fluxes across the thylakoid membranes of intact leaves (Vredenberg & Bulychev 1976) and in isolated chloroplast (Cruz *et al.* 2001) in dark to light transitions (c.f. Flores *et al.* 1983; Kramer, Dimarco & Loreto 1995; Kramer *et al.* 1999; Cruz *et al.* 2001; Kramer, Cruz & Kanazawa 2003).

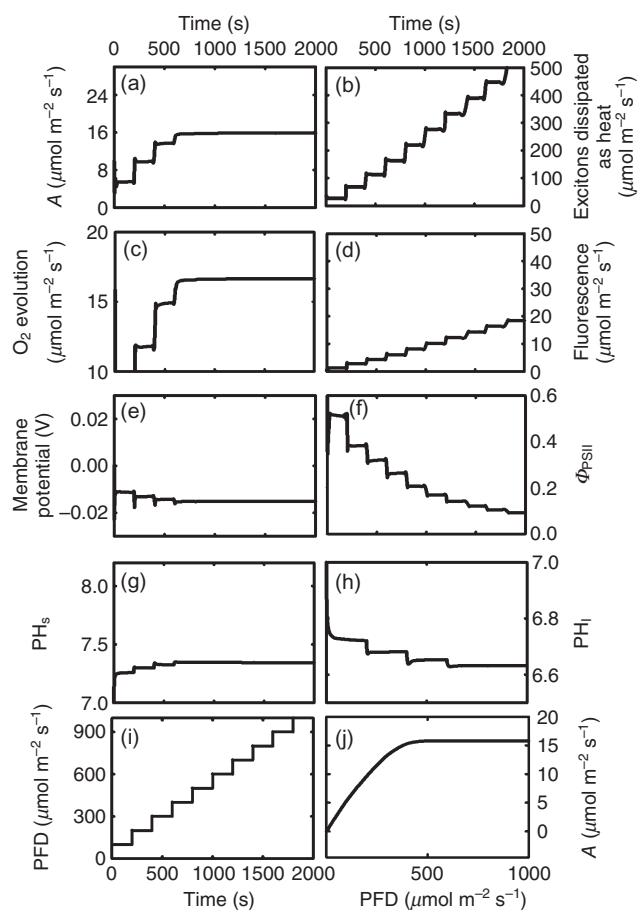


Figure 3. The predicted response of photosynthesis to photon flux density (PFD) in terms of (a) net leaf photosynthetic CO₂ uptake rate (A); (b) 'excitons' dissipated as heat, (c) the rate of O₂ evolution by photosystem II (PSII); (d) chlorophyll fluorescence; (e) membrane potential; (f) quantum yield of PSII; (g) stromal pH; and (h) luminal pH. Here, the leaf was transferred from darkness to a PFD of $100 \mu\text{mol m}^{-2} \text{s}^{-1}$, which was maintained for 200 s, and then increased by a further $100 \mu\text{mol m}^{-2} \text{s}^{-1}$, with steady state being achieved before the end of 200 s at each step. These step increases were continued at 200 s intervals until $1000 \mu\text{mol m}^{-2} \text{s}^{-1}$ was attained (panel i). A response curve of A to PFD is reconstructed from the data of panel A (panel j). The x -axis of all panels is time (s), except panel j, where the x -axis is PFD. Apart from variation in PFD, all other conditions for simulations were as in Fig. 2.

e -Photosynthesis provided realistic predictions of the responses of steady-state A to PFD (A -PFD response, Fig. 3) and to c_i (A - c_i response, Fig. 4). The A - c_i and A -PFD curves have been used extensively to probe the limitation of photosynthesis, either by RuBP carboxylation or RuBP regeneration (Farquhar *et al.* 1980). To construct the A -PFD curve (Fig. 3a), each PFD was maintained for 200 s with increments of $100 \mu\text{mol m}^{-2} \text{s}^{-1}$ from 100 to $1000 \mu\text{mol m}^{-2} \text{s}^{-1}$ (Fig. 3i). At PFD below $500 \mu\text{mol m}^{-2} \text{s}^{-1}$, steady-state A increased almost linearly with increasing PFD, consistent with a dominating RuBP regeneration limitation, in line with the widely validated steady-state biochemical model of photosynthesis of Farquhar *et al.* (1980). Beyond $500 \mu\text{mol m}^{-2} \text{s}^{-1}$, increases in

PFD resulted in only slight increases in A consistent with RuBP carboxylation rate as the major limitation to A in high light (Fig. 3a), again in line with Farquhar *et al.* (1980). With increases in PFD, the amount of energy dissipated by heat gradually increased (Fig. 3b). The predicted increased heat dissipation through NPQ is expected in order to protect PSII from damage by excessive excitation (Fig. 3b) (Long *et al.* 1994; Horton *et al.* 1996; Ort 2001).

The response of A to c_i was simulated by attaining steady-state photosynthesis at a c_i of $1000 \mu\text{mol mol}^{-1}$ and then decreasing c_i in $100 \mu\text{mol mol}^{-1}$ increments each maintained for 200 s, until c_i reached $100 \mu\text{mol mol}^{-1}$ (Fig. 4i). Consistent with the steady-state model of Farquhar *et al.* (1980), for a light-adapted leaf A declined slowly with decrease in c_i until

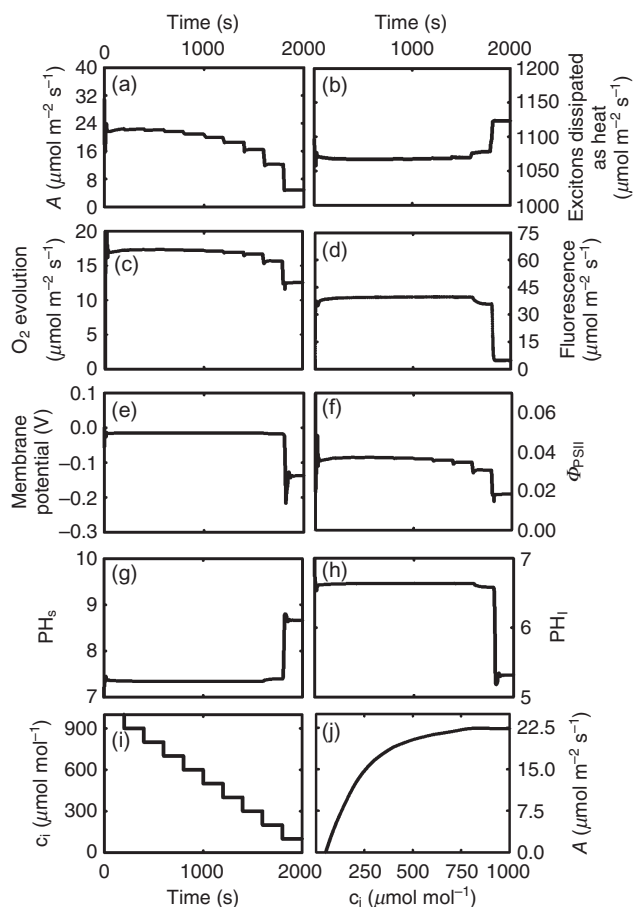


Figure 4. The predicted response of photosynthesis to intercellular CO₂ concentration (c_i) in terms of (a) net leaf photosynthetic CO₂ uptake rate (A); (b) 'excitons' dissipated as heat, (c) the rate of O₂ evolution by photosystem II (PSII); (d) chlorophyll fluorescence; (e) membrane potential; (f) photosystem II (PSII) electron transfer rate; (g) stromal pH; and (h) luminal pH. Here, the initial leaf c_i was set at $1000 \mu\text{mol mol}^{-1}$ for 200 s, and then decreased in steps of $100 \mu\text{mol mol}^{-1}$ every 200 s until $100 \mu\text{mol mol}^{-1}$ was attained (panel i). A response curve of A to c_i is reconstructed from the data of panel A (panel j). The x -axis of all panels is time (s), except panel j, where the x -axis is c_i . Apart from variation in c_i and use of a photon flux density (PFD) of $1000 \mu\text{mol m}^{-2} \text{s}^{-1}$, throughout, all other conditions for simulations were as in Fig. 2.

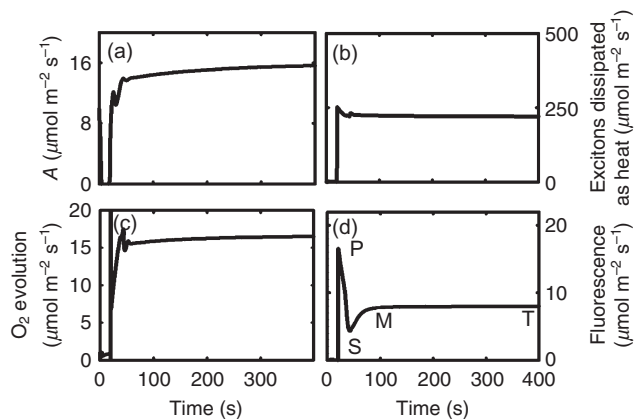


Figure 5. Simulated chlorophyll fluorescence induction and quenching, showing PMST kinetics with P representing the initial peak of fluorescence after initial illumination, S representing a semi-steady state, M representing a possible maximum fluorescence after S and T representing a terminal steady state (Papageorgiou, 1975) (panel d), and parallel changes in (a) net leaf photosynthetic CO_2 uptake rate (A); (b) heat dissipation and (c) the rate of O_2 evolution by photosystem II (PSII). The photon flux density (PFD) of the actinic light was $500 \mu\text{mol m}^{-2} \text{s}^{-1}$. Intercellular $[\text{CO}_2]$ is $280 \mu\text{mol mol}^{-1}$ and $[\text{O}_2]$ is 210mmol mol^{-1} . The measurement light PFD was $7 \mu\text{mol m}^{-2} \text{s}^{-1}$. The actinic light of $500 \mu\text{mol m}^{-2} \text{s}^{-1}$ was added at the 20th second.

about $300 \mu\text{mol mol}^{-1}$, after which A declines rapidly, reflecting the transition from RuBP-limited to RuBP-saturated photosynthesis (Fig. 4a). When photosynthesis is RuBP-limited, decrease in A with decrease in c_i results simply from increased partitioning of RuBP and electrons to C2 metabolism, which is consistent with the small change in both J_{PSII} (Fig. 4f) and O_2 evolution associated with whole-chain electron transport (Fig. 4c), followed by much larger declines at $c_i < 400 \mu\text{mol mol}^{-1}$, as CO_2 supply limitation slows the utilization of the products of whole-chain electron transport. In Fig 4a, leaf CO_2 uptake decreases more with decreases in c_i than does O_2 evolution. This is because O_2 evolution here and in other figures is simply attributed to whole-chain electron transport and is not corrected for photorespiratory and dark respiratory fluxes.

Chlorophyll fluorescence decay curve

Fluorescence induction (FI) includes both rise and decay components each of which are composed of characteristic phases (e.g. Govindjee 1995). Compared to the number of studies regarding the mechanisms of the OJIP phases of the FI rise (Stirbet *et al.* 1998; Lazar 2003; Zhu *et al.* 2005; Lazar & Schansker 2009), relatively less theoretical effort has been made to explore the mechanisms of PSMT decay phases. This is no doubt because PSMT results from a more diverse set of processes compared to the initial OJIP, and critically depends on the whole electron transfer processes and the dynamics of carbon metabolism. Since *e*-photosynthesis incorporates these processes, a critical test of the model is its ability to simulate the well established PSMT decay phase, and

simulated measurement of J_{PSII} during this phase with saturating light flashes. Previously, we have shown that the OJIP induction can be realistically simulated (Zhu *et al.* 2005), here we show a temporally realistic simulation by *e*-photosynthesis of the PSMT phase as a result of connecting PSII processes with downstream electron transport, thylakoid membrane chemical concentration and electrical potential gradients, and carbon metabolism. Transition from M to T was consistent with attainment of steady-state A , O_2 evolution associated with whole-chain electron transport and heat dissipation (Fig. 5). Fluorescence induction phases OJIPSMT can be easily and rapidly measured in intact leaves. They provide a potential means for high-throughput screening, for example, of the progeny of crosses. However, a barrier to their application has been an understanding of the relationship of these transients to factors, which actually affect productivity and environmental tolerance. *e*-Photosynthesis therefore provides a theoretical framework for determining and testing hypotheses about the underlying processes causing variation in these easily measured transients in the fluorescence induction curve.

Use of saturating pulses of light coupled with measurement of modulated chlorophyll fluorescence has emerged as the major method for determining J_{PSII} and NPQ during induction and during steady-state photosynthesis in intact

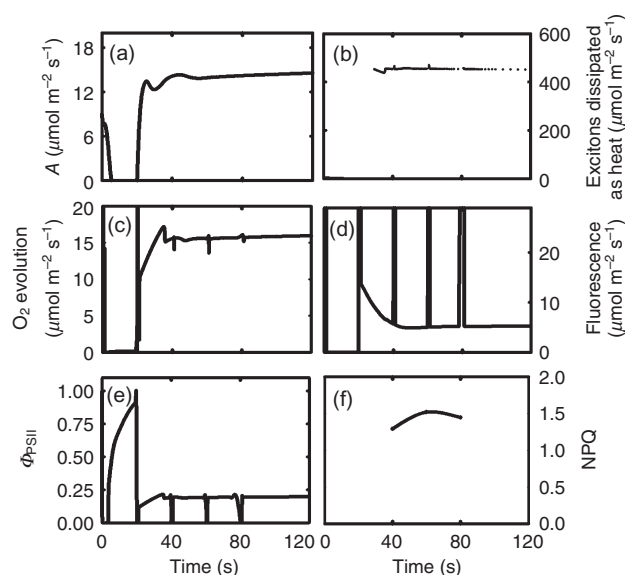


Figure 6. A simulated analysis of chlorophyll fluorescence quenching using a series of saturating flashes. A photon flux density (PFD) of $1 \mu\text{mol m}^{-2} \text{s}^{-1}$ was 'applied' between 0 and 20th second, then, a saturating pulse with PFD of $8000 \mu\text{mol m}^{-2} \text{s}^{-1}$ was 'applied' between 20 and 21st second. An actinic light with PFD of $500 \mu\text{mol m}^{-2} \text{s}^{-1}$ was 'applied' 200 s later, and saturating flashes of $8000 \mu\text{mol m}^{-2} \text{s}^{-1}$ and 1 s duration 'applied' at 5 s intervals. Intercellular $[\text{CO}_2]$ was $280 \mu\text{mol mol}^{-1}$ and $[\text{O}_2]$ is 210mmol mol^{-1} . Panels show the responses of (a) photosynthetic CO_2 uptake rate (A); (b) 'excitons' released as heat; (c) the rate of O_2 evolution by photosystem II (PSII); (d) chlorophyll fluorescence; (e) the quantum efficiency of electron transport through PSII (Φ_{PSII}); and (f) non-photochemical quenching (NPQ).

leaves. As a further test of *e*-photosynthesis, such measurements were simulated starting with application of a saturating flash to a dark-adapted leaf, and then followed by a sequence of flashes through induction of photosynthesis. This yielded temporally and quantitatively realistic patterns of the emergence of chlorophyll fluorescence quenching, NPQ, heat dissipation and Φ_{PSII} during induction of *A* following a dark-light transition (Fig. 6).

CONCLUSIONS

Photosynthesis is almost unique among biological processes in the rich array of external signals that may be measured, thereby allowing screening or imaging of large numbers of plants. Lacking, however, has been a comprehensive theoretical framework for assessing and interpreting these signals used in combination. *e*-Photosynthesis now provides a workable platform. Although this model is perhaps the most comprehensive to date, it is far from complete. Many further feedback and feedforward controls surely exist. However, the outcomes of the simulations show that the existing knowledge incorporated into this mechanistic model is sufficient to reproduce widely observed *in vivo* responses of photosynthesis to environmental perturbations. The model now provides a framework for informed engineering of improved photosynthetic efficiency. It also provides a means to interpret gas exchange, fluorescence and absorption spectroscopy more fully and from a mechanistic basis. This in turn could improve the value of these measures in the development of high-throughput screening for the emerging phenomics field. The *e*-photosynthesis model provides a critical module for a dynamic systems model of canopy photosynthesis as well (Zhu, Song & Ort 2012). Finally, as demonstrated in the sensitivity analysis, the model provides a quantitative assessment of strengths and weaknesses of current understanding of the photosynthetic system as a whole.

Inevitably improved parameters and equations representing the >100 steps of this model will be developed and complete parameter sets will become available for individual plants. To this extent, *e*-photosynthesis is intended as a 'living' model available to be improved by the community.

Availability

This model is available for research and teaching upon request from authors. The model can be freely used for academic purposes. For commercial purposes, special commercial license is required.

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SUPPORTING INFORMATION

Additional Supporting Information may be found in the online version of this article:

- Appendix S1.** List of Abbreviations and their Definitions.
Appendix S2. Tables showing the abbreviations of reaction rates, values of parameters and kinetic constants, initial concentrations of metabolites and compounds used in the model of the *e*-Photosynthesis.
Appendix S3. Equations used in *e*-Photosynthesis.

Appendix I List of Abbreviations and their Definitions

Table I.1

The definition of compounds in the stroma and lumen, and the definition of the different components of the electron transfer chain used in *e*-Photosynthesis. The column labeled as Unit shows the units used to represent the quantity of these compounds or components in *e*-Photosynthesis.

| Components | Full Name | Unit |
|-----------------------------|--|--------------------------------|
| ISPH | Iron sulfur protein | $\mu\text{mol m}^{-2}$ |
| cyt f | Cytochrome f | $\mu\text{mol m}^{-2}$ |
| Eaf | The total of Rubisco, carbamylated Rubisco, and carbamylated Rubisco bound with Mg^{2+} | mmol l^{-1} |
| ER | Rubisco bound with RuBP | mmol l^{-1} |
| ECMR | Carbamylated Rubisco bound with Mg^{2+} and RuBP | mmol l^{-1} |
| MT | Total stromal Mg^{2+} including both free form and those bound with Rubisco | mmol l^{-1} |
| C | Stromal CO_2 | mmol l^{-1} |
| [Rubisco] | Leaf Rubisco concentration | mg m^{-2} |
| [activase] | Leaf activase concentration | mg m^{-2} |
| Ax | Antheraxanthin | $\text{mmol (mol chl a)}^{-1}$ |
| Vx | Violaxanthin | $\text{mmol (mol chl a)}^{-1}$ |
| Zx | Zeaxantin | $\text{mmol (mol chl a)}^{-1}$ |
| Thio_o | Oxidized thioredoxin | mmol l^{-1} |
| Fd | Oxidized ferredoxin | mmol l^{-1} |
| Activase_o | Oxidized Rubisco activase | mmol l^{-1} |
| GADPH_o | Oxidized GAP Dehydrogenase | mmol l^{-1} |
| FBPase_o | Oxidized FBPase | mmol l^{-1} |
| SBPase_o | Oxidized SBPase | mmol l^{-1} |

| | | |
|---------------------------------------|---|----------------------|
| PRK_o | Oxidized Phosphate ribulose kinase | mmol l ⁻¹ |
| ATPase_o | Oxidized ATP synthase | mmol l ⁻¹ |
| ADPGPP_o | Oxidized ADP glucose pyrophosphatase | mmol l ⁻¹ |
| Thio_r | Reduced thioredoxin | mmol l ⁻¹ |
| Fd_r | Reduced ferredoxin | mmol l ⁻¹ |
| Activase_r | Reduced Rubisco activase | mmol l ⁻¹ |
| GADPH_r | Reduced GAP Dehydrogenase | mmol l ⁻¹ |
| FBPase_r | Reduced FBPase | mmol l ⁻¹ |
| SBPase_r | Reduced SBPase | mmol l ⁻¹ |
| PRK_r | Reduced Phosphate ribulose kinase | mmol l ⁻¹ |
| ATPase_r | Reduced ATP synthase | mmol l ⁻¹ |
| ADPGPP_r | Reduced ADP glucose pyrophosphatase | mmol l ⁻¹ |
| ISP_{ox} | Oxidized iron sulfur protein, | μmol m ⁻² |
| ISP_{ox}QH₂ | The complex of oxidized iron sulfur protein and plastoquinonol | μmol m ⁻² |
| PQH[•] | Plastosemiquinone | μmol m ⁻² |
| Cyt b_L | Low potential cytochrome b ₆ | μmol m ⁻² |
| PQ_{ib} | Plastoquinone bound to the plastoquinone reducing site of cyt b ₆ f | μmol m ⁻² |
| PQ | Free plastoquinone in thylakoid membrane | μmol m ⁻² |
| Cyt b_H | High potential cytochrome b ₆ | μmol m ⁻² |
| PQ⁻ | Plastoquinone bound at plastoquinone reducing site of cyt b ₆ f with one negative charge | μmol m ⁻² |
| PQ²⁻ | Fully reduced plastoquinol bound at plastoquinone reducing site of cyt b ₆ f | μmol m ⁻² |
| PQH₂ | Free plastoquinol in the thylakoid membrane | μmol m ⁻² |
| PC | Plastocyanin | μmol m ⁻² |
| P₇₀₀ | Reaction center of photosystem I in reduced state | μmol m ⁻² |

| | | |
|---|---|----------------------|
| ADP | ADP in stroma | mmol l ⁻¹ |
| Pi | Inorganic phosphate in stroma | mmol l ⁻¹ |
| ATP | ATP in stroma | mmol l ⁻¹ |
| K_s⁺ | K ⁺ in stroma | mmol l ⁻¹ |
| Mg_s²⁺ | Mg ²⁺ in stroma | mmol l ⁻¹ |
| Cl_s⁻ | Cl ⁻ in stroma | mmol l ⁻¹ |
| K_l⁺ | K ⁺ in lumen | mmol l ⁻¹ |
| Mg_l²⁺ | Mg ²⁺ in lumen | mmol l ⁻¹ |
| Cl_l⁻ | Cl ⁻ in lumen | mmol l ⁻¹ |
| A_{IP} | The photons on the peripheral antenna of photosystem I | μmol m ⁻² |
| U_I | Photons on the core antenna of photosystem I | μmol m ⁻² |
| A₀ | Oxidized primary electron acceptor of PSI | μmol m ⁻² |
| BFH_s | Protonated buffer species in stroma | mmol l ⁻¹ |
| BF_s⁻ | Unprotonated buffer species in stroma | mmol l ⁻¹ |
| BFH_l | Protonated buffer species in lumen | mmol l ⁻¹ |
| BF_l⁻ | Unprotonated buffer species in lumen | mmol l ⁻¹ |
| NADPH | NADPH in stroma | mmol l ⁻¹ |
| NADP | NADP in stroma | mmol l ⁻¹ |
| E.b_L.b_H | Cyt b without binding of plastoquinol or plastoquinone | μmol m ⁻² |
| E.b_L.b_H.ISP_{ox}.P | Enzyme substrate complex i.e. Cyt b bound with ISP _{ox} and PQH ₂ | μmol m ⁻² |
| QH₂ | | |
| E.b_L.b_H.PQH⁻ | Cyt b with semiplastoquinone bound | μmol m ⁻² |
| ISPH_{red} | Protonated reduced iron sulfur protein | μmol m ⁻² |
| ISPH_{ox}⁺ | Protonated oxidized iron sulfur protein | μmol m ⁻² |
| E.b_L.b_H | Enzyme cyt b ₆ with one negative charge on Cyt b _L | μmol m ⁻² |

| | | |
|---|---|----------------------|
| E_{bL}.b_H⁻ | Enzyme Cyt b ₆ with one negative charge on Cyt b _H | μmol m ⁻² |
| H⁺ | Proton | mmol l ⁻¹ |
| A₀⁻ | The reduced primary electron acceptor of photosystem I | μmol m ⁻² |
| Fd | The oxidized ferredoxin | μmol m ⁻² |
| Cyt c₁ | Cytochrome c1 in cytochrome bc ₁ complex | μmol m ⁻² |
| Cyt c₂ | Cytochrome c2 | μmol m ⁻² |
| PQ | Plastoquinone | μmol m ⁻² |
| Q_H | The protonation state of the putative chlorophyll fluorescence quenching site | Dimensionless s |
| H_{fl} | Free proton concentration in lumen | mM |
| H_{fs} | Free proton concentration in stroma | mM |
| PH_l | Luminal pH | Dimensionless s |
| PH_s | Stromal pH | Dimensionless s |
| Fd_T | Total ferredoxin (including both oxidized and reduced) | μmol m ⁻² |
| Cytb_T | Total concentration of Cytb _L or Cytb _H at both reduced and oxidized states | μmol m ⁻² |
| PQ_T | Total concentration of plastoquinone pool in thylakoid membrane | μmol m ⁻² |
| A_{0T} | Total concentration of primary electron acceptor of PSII | μmol m ⁻² |
| f_{pH} | The regulation factor of pH on v _{bf2} and v _{bf3} | Dimensionless |
| Netcharge | The net charges in stroma | Coulomb |
| Q_i | The plastoquinone binding site of cyt b ₆ f | μmol m ⁻² |
| Q_{se} | The empty Q _i site | μmol m ⁻² |

| | | |
|--------------|---------------------------------------|------------------------|
| Q_{st} | The total concentration of Q_i site | $\mu\text{mol m}^{-2}$ |
| $\Delta\Psi$ | Membrane potential | Volt |

Table I.2

Abbreviations for reaction substrates used in the C3 photosynthetic carbon metabolism model (Zhu *et al.* 2007).

| Components | Full Name | Units |
|-------------------------|--|--|
| ADPG | ADP-glucose | mmol l^{-1} |
| ADPGPP | ADP glucose pyrophosphorylase | NA |
| AT_c | Total ADP and ATP concentration in cytosol | mmol l^{-1} |
| ATPase | ATP synthase | NA ^b |
| [CO₂] | CO ₂ concentration | mol mol^{-1} or mmol l^{-1} |
| CA | Total adenylate nucleotide in the chloroplast stroma including ATP and ADP | mmol l^{-1} |
| CN | Total of NADP ⁺ and NADPH in chloroplast stroma | mmol l^{-1} |
| CP | The total concentration of phosphate in chloroplast stroma | mmol l^{-1} |
| DHAP | Dihydroxyacetone-phosphate | mmol l^{-1} |
| DPGA | 1,3-bisphosphoglycerate | mmol l^{-1} |
| E4P | Erythrose 4-phosphate | mmol l^{-1} |
| E_t | Total Rubisco concentration | mmol l^{-1} |
| F6P | Fructose 6-phosphate | mmol l^{-1} |
| FBP | Fructose 1,6-bisphosphate | mmol l^{-1} |
| F26BP | Fructose 2,6-bisphosphate | mmol l^{-1} |
| G1P | Glucose 1-phosphate | mmol l^{-1} |
| G6P | Glucose 6-phosphate | mmol l^{-1} |

| | | |
|-------------------|--|----------------------|
| GAP | Glyceraldehyde 3-phosphate | mmol l ⁻¹ |
| GAPDH | Glyceraldehyde 3-phosphate dehydrogenase | NA |
| GCA | Glycollate | mmol l ⁻¹ |
| GCEA | Glycerate | mmol l ⁻¹ |
| GDC | Glycine decarboxylase | NA |
| GLUc | Glutamate | mmol l ⁻¹ |
| GLYc | Glycine in cytosol | mmol l ⁻¹ |
| GOA | Glyoxylate | mmol l ⁻¹ |
| HexP | Hexose phosphate, includes F6P, G6P, and G1P | NA |
| GGAT | Glycine glyoxylate aminotransferase | NA |
| GSAT | Glyoxylate serine aminotransferase | NA |
| HPR | Hydroxypyruvate | mmol l ⁻¹ |
| KGc | α -ketoglutarate | mmol l ⁻¹ |
| ODE | Ordinary differential equation | NA |
| OPOP | Pyrophosphate | mmol l ⁻¹ |
| PCOP | Photosynthetic carbon oxidation pathway | NA |
| PCRC | Photosynthetic carbon reduction cycle | NA |
| PenP | Pentose phosphate including Ri5P, Ru5P, Xu5P | mmol l ⁻¹ |
| 3-PGA | 3-Phosphoglycerate | mmol l ⁻¹ |
| PGCA | 3-Phosphoglycollate | mmol l ⁻¹ |
| PRK | Ribulose-5-phosphate kinase | NA |
| PGCA Pase | Phosphoglycollate phosphotase | NA |
| PGA Kinase | 3-phosphoglycerate kinase | NA |
| Ri5P | Ribose 5-phosphate | mmol l ⁻¹ |
| PRK | Phosphoribulose kinase | mmol l ⁻¹ |
| PTc | Total phosphate concentration in cytosol | mmol l ⁻¹ |
| Ru5P | Ribulose 5-phosphate | mmol l ⁻¹ |

| | | |
|----------------------|--|----------------------|
| Rubisco | Ribulose 1,5-bisphosphate Carboxylase/Oxygenase | □ □ |
| R_t | Total RuBP concentration in stroma | mmol l ⁻¹ |
| RuBP | Ribulose 1,5-bisphosphate | mmol l ⁻¹ |
| S7P | Sedoheptulose 7-phosphate | mmol l ⁻¹ |
| SBP | Sedoheptulose 1,7-bisphosphate | mmol l ⁻¹ |
| SBPase | Sedoheptulosebisphosphatase | □ □ |
| SERc | Serine in cytosol | mmol l ⁻¹ |
| SPP | Sucrose phosphate phosphatase | □ □ |
| SPS | Sucrose phosphate synthetase | □ □ |
| TPU | Triose phosphate utilization | □ □ |
| SUCc | Sucrose in cytosol | mmol l ⁻¹ |
| SUCPc | Sucrose phosphate in cytosol | mmol l ⁻¹ |
| T3P | Triose phosphate including DHAP and GAP | mmol l ⁻¹ |
| UDPGc | Uridine diphosphate glucose | mmol l ⁻¹ |
| UDPGP | UDP glucose pyrophosphorylase | NA |
| UT | Total UDP and UTP concentration in cytosol | mmol l ⁻¹ |
| Xu5P | Xylulose 5-phosphate | mmol l ⁻¹ |

^a A suffix c was added to the name of metabolites appeared in cytosol if the metabolite also exists in stroma. For example, PGA is the phosphoglycerate in stroma; while PGAc is the phosphoglycerate in cytosol.

^b NA: Not applicable

Appendix II. Tables showing the abbreviations of reaction rates, values of parameters and kinetic constants, initial concentrations of metabolites and compounds used in the model of the *e*-Photosynthesis.

Table II.1 Definitions of the reaction rates used in the *e*-Photosynthesis model and their units.

| Abbr. | Description | Unit |
|----------------|---|--------------------------------------|
| v_{ra1} | Rate of dissociation of RuBP from Rubisco | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{ran1} | Rate of RuBP binding to Rubisco | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{ra7} | Rate of RuBP binding to ECM to form ECMR | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{ra6_1} | The rate of ECMR carboxylation | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{ra6_2} | The rate of ECMR oxygenation | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{av} | Rate of conversion from Ax to Vx | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{va} | Rate of conversion from Vx to Ax | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{az} | Rate of conversion from Ax to Zx | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{za} | Rate of conversion from Zx to Ax | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{bfn2} | The rate of NADPH generation | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| $v_{e2GADPH}$ | Rate of electron transfer from Thio_r to GADPH_o | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| $v_{e2FBPase}$ | Rate of electron transfer from Thio_r to FBPase_o | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| $v_{e2SBPase}$ | Rate of electron transfer from Thio_r to SBPase_o | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{e2PRK} | Rate of electron transfer from Thio_r to PRK_o | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| $v_{e2ATPase}$ | Rate of electron transfer from Thio_r to ATPase_o | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| $v_{e2ADPGPP}$ | Rate of electron transfer from Thio_r to ADPGPP_o | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| $v_{e2RuACT}$ | Rate of electron transfer from Thio_r to Activase_o | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| $v_{eFd2Thio}$ | Rate of electron transfer from Fd_r to Thio_o | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{s3s0} | Rate of state transition from the S_3 state to S_0 state of oxygen evolving complex | $\mu\text{mol m}^{-2} \text{s}^{-1}$ |
| v_{qb} | The rate of proton uptake for protonation of PQ^{2-} at Q_B site of PSII | $\mu\text{mol m}^{-2} \text{s}^{-1}$ |
| v_3 | The rate of exchange of PQ with Q_B^{2-} associated with Q_A | $\mu\text{mol m}^{-2} \text{s}^{-1}$ |

| | | |
|-------------|---|--------------------------------------|
| v_{3_n} | The rate of exchange of PQ with Q_B^{2-} associated with Q_A^- | $\mu\text{mol m}^{-2} \text{s}^{-1}$ |
| v_{r3} | The rate of the exchange of PQH ₂ with Q_B associated with Q_A | $\mu\text{mol m}^{-2} \text{s}^{-1}$ |
| v_{r3_n} | The rate of exchange of PQH ₂ with Q_B associated with Q_A^- | $\mu\text{mol m}^{-2} \text{s}^{-1}$ |
| v_1 | Rate of Rubisco catalyzed reaction: RuBP+CO ₂ →2PGA | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_2 | Rate of PGA Kinase catalyzed reaction PGA+ATP → ADP + DPGA | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_3 | Rate of GAP dehydrogenase catalyzed reaction DPGA+NADPH →GAP + Pi+NADP | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_5 | Rate of FBP Aldolase catalyzed reaction GAP+DHAP →FBP | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_6 | Rate of FBPase catalyzed reaction FBP→F6P+Pi | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_7 | Rate of transketolase catalyzed reaction F6P+GAP→E4P+Xu5P | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_8 | Rate of aldolase catalyzed reaction E4P+DHAP→SBP | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_9 | Rate of SBPase catalyzed reaction SBP→S7P+Pi | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{10} | Rate of transketolase catalyzed reaction S7P+GAP→Ri5P+Xu5P | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{13} | Rate of Ribulosebiphosphate kinase catalyzed reaction Ru5P+ATP→RuBP+ADP | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{16} | Rate of ATP synthase catalyzed reaction ADP+Pi→ATP | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{23} | Rate of ADP-glucose pyrophosphorylase and Starch Synthase catalyzed reaction ADPG+G _n →G _(n+1) +ADP | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| v_{31} | Rate of phosphate translocator catalyzed reaction | $\text{mmol l}^{-1} \text{s}^{-1}$ |

| | | |
|------------------|--|--------------------------------------|
| | DHAP _i →DHAP _o | |
| v ₃₂ | Rate of phosphate translocator catalyzed reaction | mmol l ⁻¹ s ⁻¹ |
| | PGA _i →PGA _o | |
| v ₃₃ | Rate of phosphate translocator catalyzed reaction | mmol l ⁻¹ s ⁻¹ |
| | GAP _i →GAP _o | |
| v ₁₁₁ | Rate of Rubisco RuBP + O ₂ → PGA + PGCA catalyzed reaction | mmol l ⁻¹ s ⁻¹ |
| v ₁₁₂ | Rate of phosphoglycolate phosphatase catalyzed reaction 2-PGCA +H ₂ O → GCA + Pi | mmol l ⁻¹ s ⁻¹ |
| v ₁₁₃ | Rate of glycerate kinase catalyzed reaction GCEA + ATP → PGA + ADP | mmol l ⁻¹ s ⁻¹ |
| v ₁₂₁ | Rate of glycolate oxidase catalyzed reaction GCA _C +O ₂ → H ₂ O ₂ +GOAc | mmol l ⁻¹ s ⁻¹ |
| v ₁₂₂ | Rate of serine glyoxylate aminotransferase catalyzed reaction GOAc +SERc → HPRc + GLYc | mmol l ⁻¹ s ⁻¹ |
| v ₁₂₃ | Rate of NADH-hydroxypyruvate reductase catalyzed reaction HPRc + NADc → NADHc + GCEAc | mmol l ⁻¹ s ⁻¹ |
| v ₁₂₄ | Rate of glutamate glyoxylate aminotransferase catalyzed reaction (GGAT) GOAc + GLUc → KGc + GLYc | mmol l ⁻¹ s ⁻¹ |
| v ₁₃₁ | Rate of Glycine decarboxylase catalyzed reaction GLYc + NADc → CO ₂ + NH ₃ + SERc +NADHc | mmol l ⁻¹ s ⁻¹ |
| v _{1T} | Rate of glycerate/glycolate transporter catalyzed reaction GCEAc ↔ GCEA | mmol l ⁻¹ s ⁻¹ |
| v _{2T} | Rate of glycerate/glycolate transporter catalyzed reaction GCAc ↔ GCA | mmol l ⁻¹ s ⁻¹ |
| v ₅₁ | Rate of FBP aldolase _c catalyzed reaction | mmol l ⁻¹ s ⁻¹ |

| | | |
|-----------------------|--|------------------------------------|
| | $\text{DHAPc} + \text{PGAc} \leftrightarrow \text{FBPc}$ | |
| v₅₂ | Rate of FBPase _c catalyzed reaction | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| | $\text{FBPc} \leftrightarrow \text{F6Pc} + \text{Pic}$ | |
| v₅₅ | Rate of UDP glucose pyrophosphorylase catalyzed reaction | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| | $\text{G1Pc} + \text{UTPc} \leftrightarrow \text{GDPc} + \text{UDPGc}$ | |
| v₅₆ | Rate of Sucrose phosphate synthase catalyzed reaction | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| | $\text{UDPGc} + \text{F6Pc} \leftrightarrow \text{SUCPc} + \text{UDPc}$ | |
| v₅₇ | Rate of sucrose phosphatase catalyzed reaction | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| | catalyzed reaction $\text{SUCPc} \leftrightarrow \text{Pic} + \text{SUCc}$ | |
| v₅₈ | Rate of fructose-2,6-bisphosphate 2-phosphatase catalyzed reaction | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| | $\text{F26BPc} \leftrightarrow \text{F6Pc} + \text{Pic}$ | |
| v₅₉ | Rate of 6-phosphofructo-2-kinase catalyzed reaction | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| | $\text{F6Pc} + \text{ATPc} \leftrightarrow \text{F26BPc} + \text{ADPc}$ | |
| v₆₀ | Rate of nucleoside-diphosphate kinase catalyzed reaction | $\text{mmol l}^{-1} \text{s}^{-1}$ |
| | $\text{ATPc} + \text{UDPc} \leftrightarrow \text{UTPc} + \text{ADPc}$ | |

Table II.2 The values of parameters and kinetic constants added to the *e*-Photosynthesis model in the light reactions of the *e*-Photosynthesis.

| Name | Description | Value | Literature |
|------------|---|---|---|
| k_{bf1} | Rate constant of formation of ISP.PQH ₂ complex | 10^6 s^{-1} | Model estimate based on quinine diffusion in thylakoid membrane |
| k_{ra1} | The rate constant of the activation of the Rubisco bound with RuBP by Rubisco activase | $0.006 \text{ mmol}^{-1} \text{ l s}^{-1}$ | Model estimate |
| k_{ran1} | Rate constant of formation of Rubisco-RuBP complex | $1.6 \times 10^{-3} \text{ mmol}^{-1} \text{ l s}^{-1}$ | Ernstsen <i>et al.</i> (1999) |
| K_{rae2} | Equilibrium constant of the Rubisco carbamylation reaction $EC \leftrightarrow E+C$ | 0.1 mmol | Mate <i>et al.</i> (1996) |
| K_{rae3} | Equilibrium constant for dissociation of Mg^{2+} from carbamylated Rubisco with bound RuBP ($ECM \leftrightarrow EC + Mg^{2+}$) | 1.6 mmol | Mate <i>et al.</i> (1996) |
| k_{ra6} | Catalytic number of RuBP carboxylation per active site of Rubisco | 2.5 | Portis (1992) |
| k_{ra7} | Rate constant of binding RuBP to ECM | $200 \text{ mmol}^{-1} \text{ l s}^{-1}$ | Model estimate |
| k_{ran7} | Rate constant of RuBP desociation from ECMR | 4.8 s^{-1} | Model estimate based on k_r |
| k_o | Michaelis Menten constant for O ₂ by ECMR | 0.448 mM | Jensen and Bahr (1977) |
| k_c | Michaelis Menten constant for CO ₂ by ECMR | 0.016 mM | Jensen and Bahr (1977) |

| | | | |
|-----------------------------|---|---|--|
| k_{av} | Rate constant of conversion from antheroxanthin (Ax) to violaxanthin (Vx) | 0.003 s ⁻¹ | Frommolt <i>et al.</i> (2001) |
| k_{va} | Rate constant of conversion from Vx to Ax | 0.012 s ⁻¹ | Frommolt <i>et al.</i> (2001) |
| k_{az} | Rate constant of conversion from Ax to zeaxanthin (Zx) | 0.002 s ⁻¹ | Frommolt <i>et al.</i> (2001) |
| k_{za} | Rate constant of conversion from Zx to Ax | 0.002 s ⁻¹ | Frommolt <i>et al.</i> (2001) |
| RC | Relaxation constant for changes in rate constant of heat dissipation regulated by xanthophylls cycle | Model variable | |
| k_{dm} | Maximum rate constant of heat dissipation of excitation energy regulated by the proportion of Zx in the sum of Ax, Vx and Zx. | Model variable | |
| k_{e2GADPH} | Rate constant of electron transfer from Thio _r to GADPH _o | 0.37 s ⁻¹ (mmol) ⁻¹ | Estimated based on Reichert <i>et al.</i> (2000) |
| k_{e2FBPase} | Rate constant of electron transfer from Thio _r to FBPase _o | 0.023s ⁻¹ (mmol) ⁻¹ | Estimated based on Laing <i>et al.</i> (1981) |
| k_{e2SBPase} | Rate constant of electron transfer from Thio _r to SBPase _o | 0.028s ⁻¹ (mmol) ⁻¹ | Estimated based on Laing <i>et al.</i> (1981) |
| k_{e2ATPase} | Rate constant of electron transfer from Thio _r to ATPase _o | 1s ⁻¹ (mM) ⁻¹ | Model estimate |
| k_{e2PRK} | Rate constant of electron transfer from Thio _r to PRK _o | 1s ⁻¹ (mM) ⁻¹ | Estimated based on Laing <i>et al.</i> (1981) |
| k_{e2RuACT} | Rate constant of electron transfer from Thio _r to Rubisco activase | 0.11s ⁻¹ (mM) ⁻¹ | Estimated based on Zhang <i>et al.</i> (2002) |

| | | | |
|-----------------|--|-------------------------------------|---|
| $k_{e2ADPGPP}$ | Rate constant of electron transfer from Thio _r to ADPGPP | $0.1\text{s}^{-1} (\text{mM})^{-1}$ | Estimated based on Ballicora <i>et al.</i> (2000) |
| $k_{eFd2Thio}$ | Rate constant of electron transfer from Fd _r to Thio _o | 10 | Model estimate |
| E_{m_FBPase} | Midpoint potential of GADPH | -305 mV | Schurmann (2003) |
| E_{m_SBPase} | Midpoint potential of FBPase | -300 mV | Schurmann (2003) |
| E_{m_GADPH} | Midpoint potential of GADPH | -340 mV | Sparla <i>et al.</i> (2002) |
| E_{m_PRK} | Midpoint potential of PRK | -295 mV | Hirasawa <i>et al.</i> (1999) |
| E_{m_ATPase} | Midpoint potential of GADPH | -280 mV | Ort and Oxborough (1992) |
| E_{m_RuACT} | Midpoint potential of Rubisco activase | -295 mV | Zhang <i>et al.</i> (2001); Schurmann (2003) |
| E_{m_ADPGPP} | Midpoint potential of ADP-glucose pyrophosphorylase | -290 mV | |
| E_{m_Fd} | Midpoint potential of PRK | -420 mV | Batie and Kamin (1984) |
| E_{m_Thiom} | Midpoint potential for thioredoxin m | -300 mV | Schurmann (2003) |
| E_{m_Thiof} | Midpoint potential for thioredoxin f | -290 mV | Schurmann (2003) |
| k_{bf2} | The rate constant for reaction $ISP_{ox}.PQH_2 \rightarrow PQH^{\cdot} + ISPH_{red}$ | 500 s^{-1} | Crofts <i>et al.</i> (2000) |
| k_{bf3} | The rate constant for reaction $PQH^{\cdot} + Cytb_L \rightarrow PQ + H^+ + Cytb_L^{\cdot-}$ | $5 \times 10^7\text{ s}^{-1}$ | Hong <i>et al.</i> (1999) |
| k_{bf4} | The rate constant for reaction $Cytb_L^{\cdot-} + Cytb_H \rightarrow Cytb_L + Cytb_H^{\cdot-}$ | $5 \times 10^7\text{ s}^{-1}$ | Hong <i>et al.</i> (1999) |
| k_{bf5} | The rate constant for reaction $Cytb_H^{\cdot-} + PQ \rightarrow PQ^{\cdot-} + Cytb_H$ | $5 \times 10^7\text{ s}^{-1}$ | Hong <i>et al.</i> (1999) |
| k_{bf6} | The rate constant for reaction | $5 \times 10^7\text{ s}^{-1}$ | Hong <i>et al.</i> (1999) |

| | | | |
|---------------------|--|--|--|
| | $\text{Cytb}_H^- + \text{PQ}^- \rightarrow \text{PQ}^{2-} + \text{Cytb}_H$ | | |
| k_{bf7} | The rate constant for PQ binding to Q_i site | 10^4 s^{-1} | Model estimate |
| k_{bf8} | The rate constant for reaction $\text{ISPH}_{\text{red}} + \text{Cytf} \rightarrow \text{ISPH}_{\text{ox}} + \text{Cytf}^-$ | 1000 s^{-1} | Fernandez-Velasco <i>et al.</i> (2001) |
| k_{bf9} | The rate constant for reaction $\text{Cytf}^- + \text{PC}^+ \leftrightarrow \text{Cytf} + \text{PC}$ | $8.3 \times 10^6 \text{ s}^{-1}$ | Chen (1989) |
| k_{bf10} | The rate constant for electron transfer from plastocyanin to P_{700} | $8 \times 10^8 \text{ s}^{-1}$ | Bowyer <i>et al.</i> (1979) |
| $V_{bf1\text{max}}$ | The maximum rate of ATP synthesis | $6 \text{ mmol l}^{-1} \text{ s}^{-1}$ | Wullschlegel (1993) |
| k_{qi} | The rate constant for protonation of PQ^{2-} | 10^3 s^{-1} | Hong <i>et al.</i> (1999) |
| P_K | Permeability constant for K^+ through thylakoid membrane | $3.6 \times 10^{-8} \text{ cm s}^{-1}$ | Pottosin and Schonknecht (1996) |
| P_{Mg} | Permeability constant for Mg^{2+} through thylakoid membrane | $3.6 \times 10^{-8} \text{ cm s}^{-1}$ | Pottosin and Schonknecht (1996) |
| P_{Cl} | Permeability constant for Cl^- through thylakoid membrane | $1.8 \times 10^{-8} \text{ cm s}^{-1}$ | Cruz <i>et al.</i> (2001) |
| k_{AU} | Rate constant for exciton transfer from peripheral antenna to core antenna | 10^{10} s^{-1} | Model estimate based on rate of excitation transfer between chlorophylls |
| k_{UA} | Rate constant for exciton transfer from peripheral antenna to core antenna | 10^{10} s^{-1} | Model estimate based on rate of excitation transfer between chlorophylls |

| | | | |
|--------------------------|--|--------------------------------------|---|
| k_f | The rate constant for fluorescence emission by excited chlorophyll | $1.3 \times 10^6 \text{ s}^{-1}$ | Lavergne and Trissl (1995); Lazar (1999) |
| k_d | Initial rate constant for heat dissipation of excitation energy in PSI | $2 \times 10^8 \text{ s}^{-1}$ | Lavergne and Trissl (1995); Brody (2002) |
| k_{f,ps1} | The rate constant for fluorescence emission by excited chlorophyll from core and peripheral antenna of PSI | 0 | Model assumption |
| k₁₅ | Rate constant for primary charge separation of PSI | 10^{10} s^{-1} | Chitnis (2001) |
| k₁₆ | The rate constant for reaction $A_0^- + Fd \leftrightarrow Fd^- + A_0$ | 10^5 s^{-1} | Chitnis (2001) |
| Em_ISP | Midpoint potential for iron sulfur protein | 310 mV | Hong <i>et al.</i> (1999) |
| Em_Cytl | Midpoint potential for Cyt b _L | -90 mV | Chen (1989) |
| Em_CytlH | Midpoint potential for Cyt b _H | 50 mV | Chen (1989) |
| Em_Cytc1 | Midpoint potential for Cyt f | 0.270 V | Chen (1989) |
| Em_Cytc2 | Midpoint potential for plastocyanin | 350 mV | Chen (1989) |
| RVA | The ratio of lumen volume to thylakoid membrane in chloroplast | $8 \times 10^{10} \text{ L cm}^{-2}$ | Vredenberg (1976); Vredenberg and Bulychev (1976) |
| K_{MIATP} | Michaelis Menten constant for ATP for $ADP+Pi \rightarrow ATP$ | 0.12 mmol l ⁻¹ | Model estimate |
| K_{MIADP} | Michaelis menten constant for ADP for $ADP+Pi \rightarrow ATP$ | 0.014 mmol l ⁻¹ | Davenport and Mccarty (1986) |
| K_{MIPI} | Michaelis Menten constant for Pi for $ADP+Pi \rightarrow ATP$ | 0.3 mmol l ⁻¹ | Aflalo and Shavit (1983) |

| | | | |
|----------------------------|--|--|--|
| HPR | The number of proton translocation through ATP synthase required for generation of 1 ATP | 4.66 | Vollmar <i>et al.</i> (2009) |
| K_{M2NADP} | Michaelis Menten constant for $Fd_r + NADP^+ + H^+ \rightarrow Fd + NADPH$ | 0.05 mM | Aliverti <i>et al.</i> (1995) |
| K_{M2NADPH} | Michaelis Menton constant for $Fd_r + NADP^+ + H^+ \rightarrow Fd + NADPH$ | 0.035 mM | Aliverti <i>et al.</i> (1995) |
| V_{2M} | The maximum rate for $Fd_r + NADP^+ + H^+ \rightarrow Fd + NADPH$ | 27.8 mmol l ⁻¹ s ⁻¹ | Model estimate based on Fridlyand and Scheibe (1999) |
| K₂ | The equilibrium constant for $Fd_r + NADP^+ + H^+ \rightarrow Fd + NADPH$ | 495 | Fridlyand and Scheibe (1999) |
| K_{bs} | Buffer capacity of stroma | 0.015 mol l ⁻¹ (pH unit) ⁻¹ | Oja <i>et al.</i> (1999); Cruz <i>et al.</i> (2001) |
| K_{bl} | Buffer capacity of lumen | 0.015 mol l ⁻¹ (pH unit) ⁻¹ | Oja <i>et al.</i> (1999); Cruz <i>et al.</i> (2001) |
| R | Gas constant | 8.314 J K ⁻¹ mol ⁻¹ | |
| T | Temperature | 298 K | |
| Q_c | The net charges in stroma | Coulomb | |
| F | Faraday Constant | 9.649 × 10 ⁴ Coulomb mol ⁻¹ | |
| k_{ro} | Maximal relaxation constant for changes in ‘rate constant’ of heat dissipation | 0.1 s ⁻¹ | Laisk <i>et al.</i> (1997) |
| k_r | Maximal relaxation constant for changes in ‘rate constant’ of heat dissipation under a particular Xstate | 0.1 s ⁻¹ | Laisk <i>et al.</i> (1997) |
| k_{dmo} | Maximum ‘rate constant’ of heat dissipation of excitation energy | 5.6×10 ⁷ s ⁻¹ | Model estimate |
| KE8 | The equilibrium constant for reaction | 0.21 | Model estimate |

| | | | |
|-----------------------|--|--|-----------------|
| | $\text{ISPH}_{\text{red}} + \text{Cyt } f \rightarrow \text{ISPH}_{\text{ox}} + \text{Cyt } f$ | | |
| KE9 | The equilibrium constant for | 22.55 | Model estimate |
| | $\text{Cyt } f + \text{PC}^+ \leftrightarrow \text{Cyt } f + \text{PC}$ | | |
| C | Membrane electrical capacity | $0.6 \times 10^{-6} \text{ F cm}^{-2}$ | Model estimate |
| k_{ra} | Rate constant for activation Rubisco by Rubisco activase | [activase]/13014 | Model estimates |

Table II.3 The Michaelis-Menten constants, inhibition constants and activation constants of the enzymes in the C3 photosynthesis carbon metabolism model (Zhu *et al.*, 2007).

| RN ^a | Reaction | Par ^b | Value Km:mM Vm: mM L ⁻¹ s ⁻¹ | Descriptio n ^d | Reference |
|-----------------|----------------------------|------------------|---|------------------------------|--|
| 1 | RuBP+CO ₂ →2PGA | K _{M11} | 0.0115 | CO ₂ | Jordan and Ogren (1981), Tcherkez <i>et al.</i> (2006) |
| 1 | RuBP+CO ₂ →2PGA | K _{M12} | 0.222 | O ₂ | Jordan and Ogren (1981), von Caemmerer (2000) |
| 1 | RuBP+CO ₂ →2PGA | K _{M13} | 0.020 | RuBP | Farquhar (1979) |
| 1 | RuBP+CO ₂ →2PGA | K _{I11} | 0.84 | PGA | Badger and Lorimer (1981) |
| 1 | RuBP+CO ₂ →2PGA | K _{I12} | 0.04 | FBP | Badger and Lorimer (1981) |
| 1 | RuBP+CO ₂ →2PGA | K _{I13} | 0.075 | SBP | Badger and Lorimer (1981) |
| 1 | RuBP+CO ₂ →2PGA | K _{I14} | 0.9 | Pi | Badger and Lorimer (1981) |
| 1 | RuBP+CO ₂ →2PGA | K _{I15} | 0.07 | NADPH | Badger and Lorimer (1981) |
| 1 | RuBP+CO ₂ →2PGA | V _{m1} | 2.93 | | Latzko et al (1981), Woodrow (1986), Geiger et al. (1999), Haake |

| | | | | | |
|---|--|-----------|-------------------------|----------------|---|
| | | | | | et al.(1999), Chen et al. (2005), Strand et al. (2000), Strand et al (1999), Tamoi et al (2006), Peterkofsky and Racher (1961), Chen et al (2005) |
| 2 | $\text{PGA} + \text{ATP} \leftrightarrow \text{ADP} + \text{DPGA}$ | K_{M21} | 0.240 | PGA | Larsson-Raznikiewicz (1967), Kopkesecundo et al. (1990) |
| 2 | $\text{PGA} + \text{ATP} \leftrightarrow \text{ADP} + \text{DPGA}$ | K_{M22} | 0.390 | ATP | Larsson-Raznikiewicz (1967), Kopkesecundo et al. (1990) |
| 2 | $\text{PGA} + \text{ATP} \leftrightarrow \text{ADP} + \text{DPGA}$ | K_{M23} | 0.23 | ADP | Lee (1982) |
| 2 | $\text{PGA} + \text{ATP} \leftrightarrow \text{ADP} + \text{DPGA}$ | K_{E2} | 7.6 $\times 10^{-4}$ | Equ. Const. | Laisk <i>et al.</i> (1989); Dietz et al (1984); Heber et al (1986) |
| 2 | $\text{PGA} + \text{ATP} \leftrightarrow \text{ADP} + \text{DPGA}$ | V_{m2} | 30.15 | | The same as V_{m1} |
| 3 | $\text{DPGA} + \text{NADPH} + \text{H}^+ \leftrightarrow \text{GAP} + \text{Pi} + \text{NADP}$ | K_{M31} | 0.004 | BPGA | Trost et al. (1993) |
| 3 | $\text{DPGA} + \text{NADPH} + \text{H}^+ \leftrightarrow \text{GAP} + \text{Pi} + \text{NADP}$ | K_{M32} | 0.100 | NADPH | Cerf (1978), Ferri et al (1978), Trost (1993), Macioszek and Anderson (1987) |

| | | | | | |
|---|--|------------------|---------------------|----------------|---|
| 3 | DPGA+NADPH +H ⁺ ↔GAP + Pi+NADP | V _{m3} | 4.04 | | The same as Vm1 |
| 4 | DHAP ↔GAP | K _{E4} | 0.05 | Equ. Const. | Bassham and Krause (1969) |
| 5 | GAP+DHAP ↔FBP | K _{M51} | 0.3 | GAP | Iwaki et al (1991) |
| 5 | GAP+DHAP ↔FBP | K _{M52} | 0.4 | DHAP | Iwaki et al (1991) |
| 5 | GAP+DHAP ↔FBP | K _{M53} | 0.02 | FBP | Brooks and Criddle (1966), Schnarrenberger and Kruger (1986) |
| 5 | GAP+DHAP ↔FBP | K _{E5} | 7.1 | Equ. Const. | Bassham and Krause (1969), Iwaki et al (1991) |
| 5 | GAP+DHAP ↔FBP | V _{m5} | 1.22 | | The same as Vm1 |
| 6 | FBP→F6P+Pi | K _{M61} | 0.033 | FBP | Charles and Halliwell (1981) |
| 6 | FBP→F6P+Pi | K _{I61} | 0.7 | F6P | Heldt (1983) |
| 6 | FBP→F6P+Pi | K _{I62} | 12 | Pi | Charles and Halliwell (1981) |
| 6 | FBP→F6P+Pi | K _{E6} | 6.7×10 ⁵ | Equ Const. | Bassham and Krause (1969) , Laisk <i>et al.</i> (1989) |
| 6 | FBP→F6P+Pi | V _{m6} | 0.734 | | The same as Vm1 |
| 7 | F6P+GAP→E4P+Xu5P | K _{M71} | 0.1 | Xu5P | Murphy and Walker (1982), Laisk <i>et al</i> (1989) |
| 7 | F6P+GAP→E4P+Xu5P | K _{M72} | 0.1 | GAP | Sprenger et al (1995), Schenk et al (1998) |

| | | | | | |
|----|---------------------------------|------------|-------------------|----------------|--|
| 7 | $F6P+GAP \rightarrow E4P+Xu5P$ | K_{M73} | 0.1 | F6P | Model estimate |
| 7 | $F6P+GAP \rightarrow E4P+Xu5P$ | K_{E7} | 10 | Equ. Const. | Bassham and Krause (1969), Laisk <i>et al.</i> (1989) |
| 7 | $F6P+GAP \rightarrow E4P+Xu5P$ | V_{m7} | 6.24 | | The same as V_{m1} |
| 8 | $E4P+DHAP \rightarrow SBP$ | K_{M8} | 0.02 | SBP | Brooks and Criddle (1966) |
| 8 | $E4P+DHAP \rightarrow SBP$ | K_{M81} | 0.4 | DHAP | Iwaki et al (1991) |
| 8 | $E4P+DHAP \rightarrow SBP$ | K_{M82} | 0.2 | E4P | Estimate |
| 8 | $E4P+DHAP \rightarrow SBP$ | K_{E8} | 1.07 | Equ. Const. | Bassham and Krause (1969) , Laisk <i>et al.</i> (1989) |
| 8 | $E4P+DHAP \rightarrow SBP$ | V_{m8} | 1.22 | | The same as V_{m1} |
| 9 | $SBP \rightarrow S7P+Pi$ | K_{M9} | 0.05 | SBP | Woodrow et al (1983), Cadet and Meunier (1988) |
| 9 | $SBP \rightarrow S7P+Pi$ | K_{I9} | 12 | Pi | Woodrow et al(1983) |
| 9 | $SBP \rightarrow S7P+Pi$ | K_{E9} | 6.7×10^5 | Equ. Const. | Bassham and Krause (1969), Laisk <i>et al.</i> (1989) |
| 9 | $SBP \rightarrow S7P+Pi$ | V_{m9} | 0.96 | | The same as V_{m1} |
| 10 | $S7P+GAP \rightarrow Ri5P+Xu5P$ | K_{M101} | 0.1 | X5P | Racher (1961), Laisk <i>et al</i> (1989) |
| 10 | $S7P+GAP \rightarrow Ri5P+Xu5P$ | K_{M102} | 0.072 | GAP | Albe (1991); Laisk <i>et al</i> (1989) |
| 10 | $S7P+GAP \rightarrow Ri5P+Xu5P$ | K_{M103} | 0.46 | S7P | Albe (1991); Laisk <i>et al</i> (1989) |

| | | | | | |
|----|---------------------------------|------------|-------|----------------|--|
| 10 | $S7P+GAP \rightarrow Ri5P+Xu5P$ | K_{M10} | 1.5 | R5P | Albe (1991); Laisk <i>et al</i> (1989) |
| 10 | $S7P+GAP \rightarrow Ri5P+Xu5P$ | K_{E10} | 1.17 | Equ. Const. | Bassham and Krause (1969), Laisk <i>et al.</i> (1989) |
| 10 | $S7P+GAP \rightarrow Ri5P+Xu5P$ | V_{m10} | 6.24 | | The same as V_{m1} |
| 11 | $Ri5P \leftrightarrow Ru5P$ | K_{E11} | 0.4 | Equ. Const. | Bassham and Krause (1969) |
| 12 | $Xu5P \leftrightarrow Ru5P$ | K_{E12} | 0.67 | Equ. Const. | Bassham and Krause, (1969) |
| 13 | $Ru5P+ATP \rightarrow RuBP+ADP$ | K_{M131} | 0.05 | Ru5P | Gardemann et al (1983), Omnaas et al (1985) |
| 13 | $Ru5P+ATP \rightarrow RuBP+ADP$ | K_{M132} | 0.059 | ATP | Laing et al (1981), Gardemann et al (1983), Omnaas et al (1985) |
| 13 | $Ru5P+ATP \rightarrow RuBP+ADP$ | K_{I131} | 2 | PGA | Gardemann et al (1983) |
| 13 | $Ru5P+ATP \rightarrow RuBP+ADP$ | K_{I132} | 0.7 | RuBP | Gardemann et al (1983) |
| 13 | $Ru5P+ATP \rightarrow RuBP+ADP$ | K_{I133} | 4 | Pi | Gardemann et al (1983) |
| 13 | $Ru5P+ATP \rightarrow RuBP+ADP$ | K_{I134} | 2.5 | ADP | Gardemann et al (1983) |
| 13 | $Ru5P+ATP \rightarrow RuBP+ADP$ | K_{E135} | 0.4 | ADP | Gardemann et al (1983) |
| 13 | $Ru5P+ATP \rightarrow RuBP+ADP$ | K_{I13} | 6846 | Equ. Const. | Bassham and Krause (1969), |

| | | | | | |
|----|--|------------|---------------------|----------------|---|
| | | | | | Laisk <i>et al.</i> (1989) |
| 13 | $\text{Ru5P}+\text{ATP}\rightarrow\text{RuBP}+\text{ADP}$ | V_{m13} | 10.81 | | The same as V_{m1} |
| 16 | $\text{ADP}+\text{P}_i\rightarrow\text{ATP}$ | K_{M161} | 0.014 | ADP | Davenport and Mccarty (1986) |
| 16 | $\text{ADP}+\text{P}_i\rightarrow\text{ATP}$ | K_{M162} | 0.3 | Pi | Aflalo and Shavit (1983) |
| 16 | $\text{ADP}+\text{P}_i\rightarrow\text{ATP}$ | K_{M163} | 0.3 | ATP | r.f. Laisk <i>et al.</i> (1989) |
| 16 | $\text{ADP}+\text{P}_i\rightarrow\text{ATP}$ | K_{E16} | 5.7 | Equ. Const. | Bassham and Krause (1969), Laisk <i>et al.</i> (1989) |
| 16 | $\text{ADP}+\text{P}_i\rightarrow\text{ATP}$ | V_{m16} | 5.47 | | The same as V_{m1} |
| 21 | $\text{F6P}\leftrightarrow\text{G6P}$ | K_{E21} | 2.3 | Equ. Const. | Bassham and Krause (1969) |
| 22 | $\text{G6P}\leftrightarrow\text{G1P}$ | K_{E22} | 0.058 | Equ. Const. | Colowick and Sutherland (1942) |
| 23 | $\text{G1P}+\text{ATP}+\text{G}_n\rightarrow\text{PP}_i+\text{ADP}+\text{G}_n$ | K_{M231} | 0.031 | G1P | Model estimate |
| | +1 | | | | |
| 23 | $\text{G1P}+\text{ATP}+\text{G}_n\rightarrow\text{PP}_i+\text{ADP}+\text{G}_n$ | K_{M232} | 0.045 | ATP | Model estimate |
| | +1 | | | | |
| 23 | $\text{G1P}+\text{ATP}+\text{G}_n\rightarrow\text{PP}_i+\text{ADP}+\text{G}_n$ | K_{M233} | 0.14 | ADPG PPi | Model estimate |
| | +1 | | | | |
| 23 | $\text{G1P}+\text{ATP}+\text{G}_n\rightarrow\text{PP}_i+\text{ADP}+\text{G}_n$ | K_{M234} | 0.8 | Equ. | Model estimate |
| | +1 | | | | |
| 23 | $\text{G1P}+\text{ATP}+\text{G}_n\rightarrow\text{PP}_i+\text{ADP}+\text{G}_n$ | K_{e23} | 7.6×10^{-3} | Const. PGA | Model estimate |
| | +1 | | | | |
| 23 | $\text{G1P}+\text{ATP}+\text{G}_n\rightarrow\text{PP}_i+\text{ADP}+\text{G}_n$ | K_{A231} | 2.3 | Pi | Model estimate |
| | +1 | | | | |
| 23 | $\text{G1P}+\text{ATP}+\text{G}_n\rightarrow\text{PP}_i+\text{ADP}+\text{G}_n$ | K_{I231} | 0.9 | | Model estimate |

| | | | | | | | |
|-----|---|--------------------|----------|------------------|--|--|--|
| | +1 | | | | | | |
| 23 | G1P+ATP+Gn→PPi+ADP+G _n | K _{Vmo} | 0.007 | | | Model estimate | |
| | +1 | | | | | | |
| 23 | G1P+ATP+Gn→PPi+ADP+G _n | V _{m23} | 0.293 | | | The same as Vm1 | |
| | +1 | | | | | | |
| 31 | P _{ext} +DHAP _i →Pi+DHAP _o | K _{M311} | 0.077 | DHAP | | Fliege et al (1978), Portis Jr. (1983) | |
| 31 | P _{ext} +DHAP _i →Pi+DHAP _o | K _{M312} | 0.63 | Pi | | Fliege et al (1978), Portis Jr. (1983) | |
| 31 | P _{ext} +DHAP _i →Pi+DHAP _o | K _{M313} | 0.74 | P _{ext} | | Fliege et al (1978), Portis Jr. (1983) | |
| 31 | P _{ext} +DHAP _i →Pi+DHAP _o | V _{m31} | 0.879 | | | Lilley et al (1977) | |
| 32 | P _{ext} +PGA _i →Pi+PGA _o | K _{M32} | 0.25 | PGA | | Fliege et al (1978), Portis Jr. (1983) | |
| 32 | P _{ext} +PGA _i →Pi+PGA _o | V _{m32} | 0.879 | | | Lilley et al (1977) | |
| 33 | P _{ext} +GAP _i →Pi+GAP _o | K _{M33} | 0.075 | GAP | | Fliege et al (1978), Portis Jr. (1983) | |
| 33 | P _{ext} +GAP _i →Pi+GAP _o | V _{m33} | 0.879 | | | Lilley et al (1977) | |
| 111 | RuBP + O ₂ → PGA + PGCA | V _{m111} | 0.24*Vm1 | | | Ueno et al (2005); Marek and Sspalding (1991); Ku et al (1991), Devi and Raghavendra (1993), Devi et al. (1995) | |
| 112 | 2-PGCA +H ₂ O → GCA + Pi | K _{M112} | 0.026 | PGCA | | Christeller and Tolbert (1978) | |
| 112 | 2-PGCA +H ₂ O → GCA + Pi | K _{I1121} | 94 | GCA, competi | | Christeller and Tolbert (1978) | |

| | | | | | | | |
|-----|--|-------------|-------|---------|-------------------|------|--|
| | | | | | | tive | |
| | | | | | | with | |
| | | | | | | PGCA | |
| 112 | $2\text{-PGCA} + \text{H}_2\text{O} \rightarrow \text{GCA} + \text{Pi}$ | K_{I1122} | 2.55 | Pi, | Christeller and | | |
| | | | | competi | Tolbert (1978) | | |
| | | | | tive | | | |
| | | | | with | | | |
| | | | | PGCA | | | |
| 112 | $2\text{-PGCA} + \text{H}_2\text{O} \rightarrow \text{GCA} + \text{Pi}$ | V_{m112} | 52.42 | | The same as Vm111 | | |
| 113 | $\text{GCEA} + \text{ATP} \rightarrow \text{PGA} + \text{ADP}$ | K_{M1131} | 0.21 | ATP | Kleczkowski et al | | |
| | | | | | (1985) | | |
| 113 | $\text{GCEA} + \text{ATP} \rightarrow \text{PGA} + \text{ADP}$ | K_{M1132} | 0.25 | GCEA | Kleczkowski et al | | |
| | | | | | (1985) | | |
| 113 | $\text{GCEA} + \text{ATP} \rightarrow \text{PGA} + \text{ADP}$ | K_{I113} | 0.36 | PGA, | Kleczkowski and | | |
| | | | | competi | Randall (1988) | | |
| | | | | tive | | | |
| | | | | with | | | |
| | | | | ATP | | | |
| 113 | $\text{GCEA} + \text{ATP} \rightarrow \text{PGA} + \text{ADP}$ | K_{E113} | 300 | Equil. | Kleczkowski et al | | |
| | | | | Const. | (1985) | | |
| 113 | $\text{GCEA} + \text{ATP} \rightarrow \text{PGA} + \text{ADP}$ | V_{m113} | 5.72 | | The same as Vm111 | | |
| 121 | $\text{GCA}_C + \text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{GOAc}$ | K_{M121} | 0.1 | GCAc | Tolbert (1981) | | |
| 121 | $\text{GCA}_C + \text{O}_2 \rightarrow \text{H}_2\text{O}_2 + \text{GOAc}$ | V_{m121} | 1.46 | | The same as Vm111 | | |
| 122 | $\text{GOAc} + \text{SERc} \rightarrow \text{HPRc} +$ GLYc | K_{M1221} | 0.15 | GOAc | Nakamura and | | |
| | | | | | Tolbert (1983) | | |
| 122 | $\text{GOAc} + \text{SERc} \rightarrow \text{HPRc} +$ GLYc | K_{M1222} | 2.7 | SERc | Nakamura and | | |
| | | | | | Tolbert (1983) | | |
| 122 | $\text{GOAc} + \text{SERc} \rightarrow \text{HPRc} +$ GLYc | K_{I1221} | 33 | GLYc, | Nakamura and | | |
| | | | | competi | Tolbert (1983) | | |

| | | | | | | |
|-----|--------------------------------|-------------|-------------------|-----------------|-----------------------------------|--|
| | | | | | tive | |
| | | | | | with | |
| | | | | | SERc | |
| 122 | GOAc + SERc → HPRc + GLYc | K_{E122} | 0.24 | Equil. | Guynn (1982) | |
| | | | | Const | | |
| 122 | GOAc + SERc → HPRc + GLYc | V_{m122} | 9.92 | | The same as Vm111 | |
| 123 | HPRc + NADc → NADHc + GCEAc | K_{M123} | 0.09 | HPRc | Kleczkowski and Edwards (1989) | |
| 123 | HPRc + NADc → NADHc + GCEAc | K_{I123} | 12 | HPRc, self | Kleczkowski and Edwards (1989) | |
| | | | | inhibitio n | | |
| 123 | HPRc + NADc → NADHc + GCEAc | K_{E123} | 2.5×10^5 | Equil. | Guynn (1982) | |
| | | | | Const. | | |
| | | V_{m123} | 10.01 | | The same as Vm111 | |
| 124 | GOAc + GLUc → KGc + GLYc | K_{M1241} | 0.15 | GOAc | Nakamura and Tolbert (1983) | |
| 124 | GOAc + GLUc → KGc + GLYc | K_{M1242} | 1.7 | GLUc | Nakamura and Tolbert (1983) | |
| 124 | GOAc + GLUc → KGc + GLYc | K_{I124} | 2 | GLYc | Calibrated | |
| | | | | competi tive | | |
| | | | | with | | |
| | | | | GLU | | |
| 124 | GOAc + GLUc → KGc + GLYc | K_{E124} | 607 | Equi. | Cooper and Meister (1972) | |
| | | | | Const. | | |
| 124 | GOAc + GLUc → KGc + GLYc | V_{m124} | 2.75 | | The same as Vm111 | |

| | | | | | |
|-------------|--|--------------------|--------|--|------------------------------|
| 131 | GLYc + NADc → CO ₂ + NH ₃ + SERc + NADHc | K _{M1311} | 6 | GLYc | Douce et al (2001) |
| 131 | GLYc + NADc → CO ₂ + NH ₃ + SERc + NADHc | K _{I1311} | 4 | SERc, competi tive with GLYc | Douce et al (2001) |
| 131 | GLYc + NADc → CO ₂ + NH ₃ + SERc + NADHc | V _{m131} | 2.49 | | The same as Vm111 |
| 101a | GCEAc → GCEA | K _{M1011} | 0.39 | GCEA | Howitz and McCarty (1986) |
| 101a | GCEAc → GCEA | K _{I1011} | 0.28 | GCA, competi tive with GCEA | Howitz and McCarty (1986) |
| 101a | GCEAc → GCEA | V _{m101a} | 1.2 | | Howitz and McCarty (1986) |
| 101b | GCA → GCAc | K _{M1012} | 0.2 | GCA | Howitz and McCarty (1985) |
| 101b | GCA → GCAc | K _{I1012} | 0.22 | GCEAc ompetiti ve with GCA | Howitz and McCarty (1985) |
| 101b | GCA → GCAc | V _{m101b} | 1.2 | | Howitz and McCarty (1986) |
| 50 | GAPc ↔ DHAPc | K _{E501} | 1/0.05 | | Bassham 1869 |
| 51 | DHAPc + PAc ↔ FBPC | K _{m511} | .020 | FBPC | Anderson et al. |

| | | | | | |
|----|-------------------------------|-------------------|--------------------|--------|---|
| | | | | | (1975) |
| 51 | DHAPc + PGAc ↔ FBPc | K _{m512} | .300 | GAPc | Iwaki et al. (1991) |
| 51 | DHAPc + PGAc ↔ FBPc | K _{m513} | .400 | DHAPc | Iwaki et al. (1991) |
| 51 | DHAPc + PGAc ↔ FBPc | K _{m514} | .014 | SBPc | Harris and Koniger (1997) |
| 51 | DHAPc + PGAc ↔ FBPc | K _{E51} | 12 | | Thomas et al. (1997) |
| 51 | DHAPc + PGAc ↔ FBPc | V _{m51} | 0.107 | | Chen et al (2005), Strand et al. (2000), Strand et al (1999), Chen et al. (2005) |
| 52 | FBPc ↔ F6Pc + Pic | K _{m521} | .0025 | FBPc | Jang et al. (2003) |
| 52 | FBPc ↔ F6Pc + Pic | K _{I521} | .7 | F6Pc | Heldt et al. (1983) |
| 52 | FBPc ↔ F6Pc + Pic | K _{I522} | 12 | Pic | Charles & Halliwell (1981) |
| 52 | FBPc ↔ F6Pc + Pic | K _{I523} | 7*10 ⁻⁵ | F26BPc | Jang et al. (2003) |
| 52 | FBPc ↔ F6Pc + Pic | K _{E52} | 6663 | | Bassham and Krause (1969) |
| 52 | FBPc ↔ F6Pc + Pic | V _{m52} | 0.064 | | The same as V _{m51} |
| 53 | F6Pc ↔ G6Pc | K _{E31} | 2.3 | | Bassham 1869 |
| 54 | G6P ↔ G1Pc | K _{E41} | 0.0584 | | Bassham 1869 |
| 55 | G1Pc + UTPc ↔ GDPc +UDPGc | K _{m551} | .14 | G1Pc | Nakano et al. (1989) |
| 55 | G1Pc + UTPc ↔ GDPc +UDPGc | K _{m552} | .1 | UTPc | Nakano et al. (1989) |
| 55 | G1Pc + UTPc ↔ GDPc +UDPGc | K _{m553} | .11 | OPOPc | Nakano et al. (1989) |
| 55 | G1Pc + UTPc ↔ GDPc + UDPGc | K _{m554} | .12 | UDPGc | Nakano et al. (1989) |
| 55 | G1Pc + UTPc ↔ | K _{E55} | 0.31 | Equi | Lunn and Rees |

| | | | | | | |
|-----------|------------------------|-------------------|-------|---------|--|-----------------------|
| | GDPc+UDPGc | | | | | (1990) |
| 55 | G1Pc + UTPc ↔ | V _{m55} | 0.115 | | | The same as Vm51 |
| | GDPc+UDPGc | | | | | |
| 56 | UDPGc + F6Pc ↔ SUCPc + | K _{m561} | 0.8 | F6Pc | | Lunn and Rees |
| | UDPc | | | | | (1990) |
| 56 | UDPGc + F6Pc ↔ SUCPc + | K _{m562} | 2.4 | UDPGc | | Lunn and Rees |
| | UDPc | | | | | (1990) |
| 56 | UDPGc + F6Pc ↔ SUCPc + | K _{i561} | .7 | UDPc | | Harbron et al. (1981) |
| | UDPc | | | | | |
| 56 | UDPGc + F6Pc ↔ SUCPc + | K _{i562} | .8 | FBPc | | Harbron et al. (1981) |
| | UDPc | | | | | |
| 56 | UDPGc + F6Pc ↔ SUCPc + | K _{i563} | 0.4 | SUCPc | | Harbron et al. (1981) |
| | UDPc | | | | | |
| 56 | UDPGc + F6Pc ↔ SUCPc + | K _{i564} | 11 | Pic | | Harbron et al. (1981) |
| | UDPc | | | | | |
| 56 | UDPGc + F6Pc ↔ SUCPc + | K _{i565} | 50 | Sucrose | | Salerno and Pontis |
| | UDPc | | | | | (1978) |
| 56 | UDPGc + F6Pc ↔ SUCPc + | K _{E56} | 10 | Equil. | | Lunn and Rees |
| | UDPc | | | Const. | | (1990) |
| 56 | UDPGc + F6Pc ↔ SUCPc + | V _{m56} | 0.056 | | | The same as Vm51 |
| | UDPc | | | | | |
| 57 | SUCPc ↔ Pic + SUCc | K _{m571} | .35 | SUCPc | | Whitaker (1984) |
| 57 | SUCPc ↔ Pic + SUCc | K _{i572} | 10 | SUCc | | Whitaker (1984) |
| 57 | SUCPc ↔ Pic + SUCc | K _{E57} | 780 | Equil. | | Lunn and Rees |
| | | | | Const. | | (1990) |
| 57 | SUCPc ↔ Pic + SUCc | V _{m57} | 0.56 | | | The same as Vm51 |
| 58 | F26BPc ↔ F6Pc + Pic | K _{m581} | .032 | F26BPc | | Macdonald et al. |
| | | | | | | (1989) |
| 58 | F26BPc ↔ F6Pc + Pic | K _{i581} | .1 | F6Pc | | Villadsen and Nielsen |

| | | | | | |
|----|---|------------|------------------|---------|--------------------------------------|
| | | | | | (2001) |
| 58 | $F26BPc \leftrightarrow F6Pc + Pic$ | K_{I582} | .5 | Pic | Villadsen and Nielsen (2001) |
| 58 | $F26BPc \leftrightarrow F6Pc + Pic$ | V_{m58} | 0.017 | | The same as Vm51 |
| 59 | $F6Pc + ATPc \leftrightarrow F26BPc + ADPc$ | K_{m591} | 5 | ATPc | Walker and Huber (1987) |
| 59 | $F6Pc + ATPc \leftrightarrow F26BPc + ADPc$ | K_{m592} | .021 | F26BPc | Garcia de Frutos and Baanante (1995) |
| 59 | $F6Pc + ATPc \leftrightarrow F26BPc + ADPc$ | K_{m593} | 0.55 | F6Pc | Walker and Huber (1987) |
| 59 | $F6Pc + ATPc \leftrightarrow F26BPc + ADPc$ | K_{I591} | .16 | ADPc | Kretschmer and Hofmann (1984) |
| 59 | $F6Pc + ATPc \leftrightarrow F26BPc + ADPc$ | K_{I592} | 0.7 | DHAPc | Markham and Kruger (2002) |
| 59 | $F6Pc + ATPc \leftrightarrow F26BPc + ADPc$ | K_{E59} | 590 | | Cornish-Bowden (1997) |
| 59 | $F6Pc + ATPc \leftrightarrow F26BPc + ADPc$ | V_{m59} | 0.03 | | Villadsen and Nielsen (2001) |
| 60 | $ATP+UDP \leftrightarrow ADP+UTP$ | K_{m601} | 0.042 | ADPc | Kimura and Shimada (1988) |
| 60 | $ATP+UDP \leftrightarrow ADP+UTP$ | K_{m602} | 1.66 | ATPc | Kimura and Shimada (1988) |
| 60 | $ATP+UDP \leftrightarrow ADP+UTP$ | K_{m603} | 0.28 | UDPc | Jong and Ma (1991) |
| 60 | $ATP+UDP \leftrightarrow ADP+UTP$ | K_{m604} | 16 | UTPc | Fukuchi et al (1994) |
| 60 | $ATP+UDP \leftrightarrow ADP+UTP$ | K_{E60} | 16 | Equili. | Lynn and Guynn (1978) |
| 60 | $ATP+UDP \leftrightarrow ADP+UTP$ | | 6.1 | | Villadsen and Nielsen (2001) |
| 61 | $SUCPc \leftrightarrow SUCc + Pic$ | K_{E61} | $1.2 \cdot 10^7$ | Equili. | Flodgaard and Fleron |

| | | | | | |
|-----------|------------------------------------|------------|------|---------|-----------------------|
| | | | | | (1974) |
| 61 | SUCPc \leftrightarrow SUCc + Pic | V_{m61} | 1000 | | Model estimate |
| 62 | SUCc \leftrightarrow Sink | K_{m621} | 5 | Sucrose | Weschke et al. (2000) |
| 62 | SUCc \leftrightarrow Sink | V_{m62} | 2 | | Model estimate |

^a RN: Reaction number corresponding to the number in Fig. 1.

^b Parameters beginning K_M represent the Michaelis-Menten constant of the metabolite listed in the *description* column

Parameters beginning with K_I represent the inhibition constant of the inhibitor listed in the *description* column.

Parameters beginning with K_A represent the activation constant of the activator listed in the *description* column.

^c The units of the equilibrium constant are mM (which is equivalent to mmol l^{-1}) for all constants, except K_e . The unit of K_e for reactions with one substrate and one product, or reactions with two substrates and two products is dimensionless. The unit of K_e for reactions with one substrate and two products is mM. The unit for reactions with two substrates and one product is $(\text{mM})^{-1}$.

^d The description column lists the compounds to which the kinetic constant applies.

Table II.4 The initial concentrations of solutes in the stroma and lumen, and the amount of the different components of the electron transfer chain in the dark assumed in the model of electron transfer. The [ADP], [Pi] and [ATP] in the stroma are based on measurements for barley (Igamberdiev et al. 2001). The experimentally measured chloroplastic [Mg²⁺], [K⁺], and [Cl⁻] are used as the basis for estimating the stromal concentration of these ions in the dark (Gimmler 1974; Barber 1976; Schroppelmeier and Kaiser 1988). The model assumes total concentrations of stoma and luminal buffer species following Laisk et al. (1997). The [NADPH] and [NADP⁺] in the stroma are based on the measurements of (Giersch et al. 1980) and (Pettersson and Ryde-Pettersson 1988). In addition to [K⁺], [Mg²⁺], and [H⁺], the stromal concentration of cations that cannot permeate the thylakoid membrane was assumed to be 1.4 mmol l⁻¹. As a simplification, the model currently assumes that the cross-membrane electrical potential was 0 in the dark and the pH of lumen and stroma were both 7. The initial concentrations of components around PSII are described in detail in the model of fluorescence induction (Zhu *et al* 2005).

| Components | Conc. | Unit |
|-----------------------------|--------------|--------------------------------|
| ISPH | 0 | μmol m ⁻² |
| cyt f | 1 | μmol m ⁻² |
| Eaf | 0 | mmol l ⁻¹ |
| ER | 0.3 | mmol l ⁻¹ |
| ECMR | 0 | mmol l ⁻¹ |
| MT | 5 | mmol l ⁻¹ |
| C | 0.012 | mmol l ⁻¹ |
| Rubisco | 1072 | mg m ⁻² |
| Rubisco activase | 80 | mg m ⁻² |
| Ax | 10 | mmol (mol chl a) ⁻¹ |
| Vx | 160 | mmol (mol chl a) ⁻¹ |
| Zx | 5 | mmol (mol chl a) ⁻¹ |
| Thio_o | 0.081 | mmol l ⁻¹ |
| Fd_o | 0.081 | mmol l ⁻¹ |
| Activase_o | 0.0056 | mmol l ⁻¹ |
| GADPH_o | 0.0033 | mmol l ⁻¹ |

| | | |
|---------------------------------------|---------|----------------------|
| FBPase_o | 0.003 | mmol l ⁻¹ |
| SBPase_o | 0.0004 | mmol l ⁻¹ |
| PRK_o | 0.293 | mmol l ⁻¹ |
| ATPase_o | 0.0036 | mmol l ⁻¹ |
| ADPGPP_o | 0.048 | mmol l ⁻¹ |
| Thio_r | 0 | mmol l ⁻¹ |
| Fd_r | 0 | mmol l ⁻¹ |
| Activase_r | 0 | mmol l ⁻¹ |
| GADPH_r | 0 | mmol l ⁻¹ |
| FBPase_r | 0 | mmol l ⁻¹ |
| SBPase_r | 0 | mmol l ⁻¹ |
| PRK_r | 0 | mmol l ⁻¹ |
| ATPase_r | 0 | mmol l ⁻¹ |
| ADPGPP_r | 0 | mmol l ⁻¹ |
| ISP_{ox} | 1 | μmol m ⁻² |
| ISP_{ox}QH₂ | 0 | μmol m ⁻² |
| PQH[•] | 0 | μmol m ⁻² |
| Cyt b_L | 1 | μmol m ⁻² |
| PQ_{ib} | 0 | μmol m ⁻² |
| PQ | 1 | μmol m ⁻² |
| Cyt b_H | 1 | μmol m ⁻² |
| PQ[•] | 0 | μmol m ⁻² |
| PQ^{2•} | 0 | μmol m ⁻² |
| PQH₂ | 5 | μmol m ⁻² |
| PC | 1 | μmol m ⁻² |
| P₇₀₀ | 0.5 | μmol m ⁻² |
| ADP | 0.82 | mmol l ⁻¹ |
| Pi | 0.9 | mmol l ⁻¹ |
| ATP | 0.68 | mmol l ⁻¹ |
| K_s⁺ | 10 | mmol l ⁻¹ |
| Mg_s²⁺ | 5 | mmol l ⁻¹ |
| Cl_s⁻ | 1 | mmol l ⁻¹ |
| K₁⁺ | 10 | mmol l ⁻¹ |
| Mg₁²⁺ | 5 | mmol l ⁻¹ |
| Cl₁⁻ | 1 | mmol l ⁻¹ |
| A_{IP} | 0 | μmol m ⁻² |
| U_I | 0 | μmol m ⁻² |
| A₀ | 1 | μmol m ⁻² |
| Fd_r | 0.3 | μmol m ⁻² |
| BFH_s | 19.0001 | mmol l ⁻¹ |
| BFT_s | 38 | mmol l ⁻¹ |
| BFH₁ | 19.0001 | mmol l ⁻¹ |
| BFT₁ | 38 | mmol l ⁻¹ |
| NADPH | 0.21 | mmol l ⁻¹ |

| | | |
|---|------------------|----------------------|
| NADP | 0.79 | mmol l ⁻¹ |
| E.b_L.b_H | 1 | μmol m ⁻² |
| E.b_L.b_H.ISP_{ox}.PQH₂ | 0 | μmol m ⁻² |
| E.b_L.b_H.PQH[·] | 0 | μmol m ⁻² |
| ISPH_{red} | 0 | μmol m ⁻² |
| ISPH⁺_{ox} | 1 | μmol m ⁻² |
| E.b_L.b_H[·] | 0 | μmol m ⁻² |
| E.b_L.b_H⁻ | 0 | μmol m ⁻² |
| H⁺ | 10 ⁻⁴ | mmol l ⁻¹ |
| A₀⁻ | 0 | μmol m ⁻² |
| Fd | 0.7 | μmol m ⁻² |
| Cyt f | 1 | μmol m ⁻² |
| PC | 1 | μmol m ⁻² |
| PQ | 1 | μmol m ⁻² |
| Q_H | 0.031 | Dimensionless |
| H_{fl} | 10 ⁻⁴ | mmol l ⁻¹ |
| H_{fs} | 10 ⁻⁴ | mmol l ⁻¹ |
| Fd_T | 1 | μmol m ⁻² |
| Cytb_T | 1 | μmol m ⁻² |
| PQ_T | 8 | μmol m ⁻² |
| A_{0T} | 1 | μmol m ⁻² |
| f_{pH} | NA | Dimensionless |
| Netcharge | 0 | Coulomb |
| Q_i | 1 | μmol m ⁻² |
| Q_{se} | NA | μmol m ⁻² |
| Q_{st} | NA | μmol m ⁻² |
| ΔΨ | 0 | V |

Table II.5 The concentrations of different metabolites used in the carbon metabolism model (Zhu *et al.*, 2007). The ranges of values found in the literature are given in the adjacent column together with their sources.

| Metabolite name | Location | Concentration (mmol l ⁻¹) | Reference |
|-----------------|----------|---------------------------------------|---|
| RuBP | Chl | 2.000 | Bassham and Krause (1969), Dietz and Heber (1984), Schimkat et al (1990), Woodrow and Mott (1993) |
| PGA | Chl | 2.400 | Schimkat et al (1990), Woodrow and Mott (1993) |
| DPGA | Chl | 0.0011 | Dietz and Heber (1984), Woodrow and Mott (1993) |
| GAP | Chl | 0.02 | Bassham and Krause (1969), Dietz and Heber (1984), Woodrow and Mott (1993) |
| DHAP | Chl | 0.48 | Bassham and Krause (1969), Dietz and Heber (1984), Schimkat et al (1990) |
| FBP | Chl | 0.670 | Bassham and Krause (1969), Dietz and Heber (1984), Schimkat et al (1990), Woodrow and Mott (1993) |
| E4P | Chl | 0.050 | Bassham and Krause (1969), Woodrow and Mott (1993) |
| S7P | Chl | 2.0 | Bassham and Krause (1969), Woodrow and Mott (1993) |
| SBP | Chl | 0.30 | Bassham and Krause (1969), Schimkat et al (1990), Woodrow and Mott (1993) |
| ATP | Chl | 0.68 | Bassham and Krause (1969), Woodrow and Mott (1993), Igamberdiev et al (2001) |

| | | | |
|------------------------|------|-------|---|
| NADPH | Chl | 0.21 | Giersch et al (1980), Woodrow and Mott (1993) |
| CO₂ | Chl | 0.012 | Dietz and Heber (1984) |
| O₂ | Chl | 0.26 | Model estimate |
| HexP | Chl | 2.2 | Schimkat et al (1990), Woodrow and Mott (1993), Winter et al (1994) |
| PenP | Chl | 0.25 | Bassham and Krause (1969), Schimkat et al (1990), Woodrow and Mott (1993) |
| Pi | Chl | 5 | Dietz and Heber (1984), Schimkat et al (1990), Woodrow and Mott (1993) |
| CP | Chl | 15 | Lilley et al (1977) |
| CA | Chl | 1.5 | Igamberdiev et al (2001) |
| CN | Chl | 0.5 | Giersch et al (1980), |
| P_{ext} | Chl | 0.5 | Bligny et al (1990), Woodrow and Mott (1993) |
| NADH | Chl | 0.22 | This was kept constant in the preliminary model |
| NADHc | Cyto | 0.47 | As for NADH |
| NAD | Chl | 0.08 | As for NADH |
| NADc | Cyt | 0.4 | As for NADH |
| ATP | Chl | 0.68 | |
| ATPc | Cyt | 0.35 | As for NADH |
| ADP | Chl | 0.82 | |
| ADPc | Cyt | 0.64 | As for NADH |
| GLUc | Cyt | 24 | As for NADH |
| KGc | Cyt | 0.4 | As for NADH |
| Pic | Chl | 5 | As for NADH |
| SERc | Cyt | 7.5 | |
| GLYc | Cyt | 1.8 | |
| PGA | Chl | 4.3 | |

| | | | |
|---------------|-----|--------------------|---|
| GOAc | Cyt | 0.028 | 30 μ l cytosol per mg chlorophyll |
| GCA | Chl | 0.36 | |
| GCAc | Cyt | 0.36 | |
| PGCA | Chl | 0.0029 | Based on the Michaelis- Menton equation for reaction 112 ^b |
| HPRc | Cyt | 0.0035 | Based on the Michaelis-Menton equation for reaction 123 ^b |
| GCEA | Chl | 0.1812 | Based on the Michaelis- Menton equation for reaction 113 ^b |
| GCEAc | Cyt | 0.1812 | Assume equilibrium with stromal Glycerate concentration |
| TPc | Cyt | 2.3 | Stitt et al. (1980), Stitt et al. (1985), Gerhardt et al. (1987), Laisk et al. (1989) |
| FBPc | Cyt | 2 | As above |
| F26BPc | Cyt | 7×10^{-6} | As above |
| UTc | Cyt | 1 | As above |
| HexPc | Cyt | 6 | As above |
| UDPG | Cyt | 0.6 | As above |
| PTc | Cyt | 15 | As above |
| ATc | Cyt | 1 | As above |

Comment: ^a Chl: chloroplast stroma; Mit: Mitochondrion; Cyt: Cytosol

Table II.6 Molecular weight and catalytic number of the enzymes in photosynthetic carbon metabolism

| Enzyme Name | EC | Molecular Weight (D) | Catalytic number¹ (s⁻¹) | Reference |
|--------------------------------|-----------|-----------------------------|--|---|
| Rubisco | 4.1.1.39 | 588000 | 2* | Spreitzer and Salvucci (2002) |
| PGA Kinase | 2.7.2.3 | 45000 | 540 | Fifis and Scopes (1978), Bentahir et al (2000) |
| GAP Dehydrogenase | 1.2.1.12 | 180000 | 50 | Speranza and Ferri (1982) |
| Aldolase | 4.1.2.13 | 7000 | 65 | Krueger and Sschnarrenberger (1983), Moorhead and Pplaxton (1990) |
| FBPase | 3.1.3.11 | 160000 | 22.9 | Tang et al. (2000), Reichert et al.(2000) |
| Transketolase | 2.2.1.1 | 160000 | 69 | Nilsson et al (1998) Teige et al. (1989) |
| SBPase | 3.1.3.37 | 66000 | 81 | Cadet et al. (1988), Cadet and Meunier (1987) |
| PRK | 2.7.1.19 | 90000 | 615 | Surek et al. (1985), Porter et al. (1986) |
| ADPG Pyrophospho-rylase | 2.7.7.27 | 210000 | 546 | Kleczkowski et al. (1991), Li and Preiss(1992) |

| | | | | |
|--|-----------|--------|------|---|
| Phosphoglycolate phosphatase | 3.1.3.18 | 100000 | 292 | Kim et al. (2004), Kerr and Gear (1974) |
| Glycerate Kinase | 2.7.1.31 | 47000 | 200 | Kleczkowski et al. (1985), Kleczkowski and Randall (1988) |
| Glycolalate oxidase | 1.1.1.79 | 125000 | 437 | Kleczkowski et al. (1986), Zelitch(1955) |
| Serine Glyoxylate aminotransferase | 2.6.1.45 | 85000 | 97 | Ireland and Joy (1983), Paszkowski and Niedzielsa (1990) |
| Glycerate dehydrogenase | 1.1.1.29 | 90000 | 1629 | Julliard and Breton-Gilet (1997), Izumi et al.(1990) |
| Glutamate Glyoxylate aminotransferase | 2.6.1.44 | 70800 | 54 | Paszkowski and Niedzielska (1989) |
| Glycine decarboxylase | 1.4.4.2 | 270000 | 18 | Hiraga and Kikuchi (1980), Kochi and Kikuchi (1974) |
| 6-phosphofructo-2-k inase | 2.7.1.105 | 390000 | 9300 | Villadsen and Nielsen (2001), Baez et al. (2003) |
| fructose-2,6-bisphos phate 2-phosphatase | 3.1.3.46 | 390000 | 1550 | Pilkis et al. (1987), Villadsen and Nielsen (2001), |
| UDP Glucose | 2.7.7.9 | 53000 | 400 | Gustafson and |

| | | | | |
|---------------------------------------|----------|--------|------|---|
| pyrophosphorylase | | | | Gander (1972), Sowokinos et al (1993) |
| Sucrose phosphate synthase | 2.4.1.14 | 480000 | 640 | Sonnewald et al. (1993) |
| Sucrose phosphatase | 3.1.3.24 | 120000 | 2500 | Echeverria and Salerno (1994), Lunn et al. (2000) |

Equations used in *e*-Photosynthesis

Section 1.1 Additional rate equations used in *e*-Photosynthesis in addition to those in Zhu et al (2005) and Zhu *et al.* (2007). The model of electron transfer extends the model of fluorescence induction (Zhu et al. 2005) where the detailed lists of rate equations for excitation and electron transfer around PSII is provided. The additional rate equations for the excitation energy and electron transfer processes around PSI, the modified Q cycle, nonphotochemical quenching, ion transfer between lumen and stroma, ATP and NADPH synthesis, and regulatory mechanisms are listed following.

$$V_{\text{bfl}} = V_{\text{max1}} \left(\frac{[\text{ISP}_{\text{ox}}]}{([\text{ISP}_{\text{(ox)}}] + [\text{ISPH}_{\text{(red)}}])} \frac{[\text{PQH}_2]}{([\text{PQ}] + [\text{PQH}_2] + [\text{PQH}])} \right) \dots \dots (1)$$

$$V_{\text{max1}} = k_{\text{bfl}} ([\text{ISP}_{\text{ox}}] + [\text{ISPH}_{\text{red}}]) \dots \dots (2)$$

$$[\text{ISP}_{\text{ox}}] = \frac{[\text{ISP}_{\text{ox}}]}{1 + \frac{[\text{H}^+]}{[10^{-\text{pK}}]}} \dots \dots (3)$$

$$\text{Temp1} = 10^{(5.5-8)} \dots \dots (4)$$

$$a = \frac{\text{Temp1}}{1 + \text{Temp1}} \dots \dots (5)$$

$$\text{Temp2} = 10^{(5.5-\text{pH}_1)} \dots \dots (6)$$

$$b = \frac{\text{Temp2}}{1 + \text{Temp2}} \dots \dots (7)$$

$$f_{\text{pH}} = 1 - (b - a) \dots \dots (8)$$

$$v_{bf2} = k_{bf2} [PQH_2 \cdot ISP_{ox}] f_{pH} \dots \dots (9)$$

$$v_{bf3} = k_{bf3} f_{pH} [PQH] \frac{[Cytb_L]}{[Cytb_T]} \dots \dots (10)$$

$$v_{bf4} = k_{bf4} [Cytb_L^-] \frac{[Cytb_H]}{[Cytb_T]} \dots \dots (11)$$

$$v_{bf5} = k_{bf5} [Cytb_H^-] \frac{[PQ_{nb}]}{[Cytb_T]} \dots \dots (12)$$

$$v_{bf6} = k_{bf6} [Cytb_H^-] \frac{[PQ^-]}{[Cytb_T]} \dots \dots (13)$$

$$\text{where } [Cytb_T] = [Cytb_L] + [Cytb_L^-] \dots \dots (14)$$

$$v_{bf7} = k_{bf7} [Cytb_T] \frac{[Q_{se}^-] [PQ]}{[Q_{sT}] [PQ_T]} \dots \dots (15)$$

$$KE8 = e^{\frac{(-Em_{Cyt f} - Em_{ISP}) (-9649) 10^4}{RT}} \dots \dots (16)$$

$$v_{bf8} = k_{bf8} [Cytb_T] \left(\frac{[ISPH_{red}] [Cyt f]}{[Cytb_T]^2} - \frac{[ISP_{ox}] [Cyt f^-]}{[Cytb_T]^2 KE8} \right) f_{pH} \dots \dots (17)$$

$$KE9 = e^{\frac{(-Em_{PC} - Em_{Cyt f}) (-9,649) 10^4}{RT}} \dots \dots (18)$$

$$v_{bf9} = k_{bf9} [Cytb_T] \left(\frac{[PC^+] [Cyt f^-]}{[Cytb_T]^2} - \frac{[Cyt f] [PC]}{[Cytb_T]^2 KE9} \right) \dots \dots (19)$$

$$v_{bf10} = k_{bf10} \left(\frac{[PC] [P_{700}^+]}{P_{700T}} - \frac{[PC^+] [P_{700}]}{P_{700T} K_{10}} \right) \dots \dots (20)$$

$$v_{bf11} = \frac{V_{bf11max} ([ADP] [Pi] - \frac{[ATP]}{kE})}{(K_{mADP} K_{mP}) \left(1 + \frac{[ADP]}{K_{mADP}} + \frac{[Pi]}{K_{mP}} + \frac{[ATP]}{K_{mATP}} + \frac{[ADP] [Pi]}{K_{mADP} K_{mP}} \right)} \dots \dots (21)$$

$$kE = \exp(-\Delta G/RT) \dots \dots (22)$$

$$\Delta G = \Delta G^\circ + 0.592 \text{ HPR} \ln([H_{f1}]/[H_{fs}]) + \text{HPR} \Delta \Psi F \dots \dots (23)$$

$$v_{qi} = 2k_{qi} [Q^2] f_{pH2} \dots \dots (24)$$

$$f_{pH2} = (25.359 - 0.0425 \text{ pHs}^3 + 1.0986 \text{ pHs}^2 - 9.183 \text{ pHs})/0.72 \dots \dots (25)$$

$$v_{IPC} = [A_{IP}] k_{AU} \dots \dots (26)$$

$$v_{ICP} = [U_I] k_{UA} \dots\dots (27)$$

$$v_f = ([A_{IP}] + [U_I]) k_{f,psi} \dots\dots (28)$$

$$v_d = ([A_{IP}] + [U_I]) k_d \dots\dots (29)$$

$$v_{qb} = 2(v_3 - v_{r3} + v_{3_n} - v_{r3_n}) \dots\dots (30)$$

where equations for v_3 , v_{r3} , v_{3_n} and v_{r3_n} describing reactions associated around photosystem II and are defined in Appendix 2 of Zhu et al (2005)

$$v_{inc} = I_{in} \frac{200 \cdot 80}{(200 + 290) 200} \dots\dots (31)$$

$$v_{inp} = I_{in} \frac{200 \cdot 120}{(200 + 290) 200} \dots\dots (32)$$

$$v_{fp} = k_{f,ps1} [A_{ip}] \dots\dots (33)$$

$$v_{fc} = k_{f,ps1} [U_I] \dots\dots (34)$$

$$\text{NetCharge} = ([H_s^+] + [K_s^+] + 2[Mg_s^{2+}] - [OH_s^-] - [Cl_s^-] - [BF_s^-] + 1.4) / 1000 \times \text{RVA} \times 6.022 \times 10^{23} \times 1.6 \times 10^{-19} \dots\dots (35)$$

$$\Delta\Psi = 2\text{NetCharge} / C \dots\dots (36)$$

$$\text{temp} = -F \Delta\Psi / RT \dots\dots (37)$$

$$v_{bf12} = P_K \frac{\text{temp}}{10} \frac{[K_1^+] - [K_s^+] e^{-\text{temp}}}{1 - e^{-\text{temp}}} / \text{RVA} \dots\dots (38)$$

$$v_{bf13} = P_K \frac{\text{temp}}{20} \frac{[Mg^{2+}_1] - [Mg^{2+}_s] e^{-\frac{\text{temp}}{2}}}{1 - e^{-\frac{\text{temp}}{2}}} / \text{RVA} \dots\dots (39)$$

$$v_{bf14} = -P_{Cl} \frac{\text{temp}}{10} \frac{[Cl_1^-] - [Cl_s^-] e^{\text{temp}}}{1 - e^{\text{temp}}} / \text{RVA} \dots\dots (40)$$

$$[P_{700e}] = [U_I] \frac{([P_{700T}] - [P_{700}^+])}{120} \dots\dots (41)$$

$$v_{bf15} = k_{15} [P_{700e}] \frac{[A_0]}{[A_{0T}]} \dots\dots (42)$$

$$v_{bf16} = k_{16} [A_0^-] \frac{[Fd]}{[Fd_T]} \dots\dots (43)$$

$$v_{bf2} = \frac{V_{2M} \left(\frac{[Fd_r]}{[Fd_T]} [NADP^+] - \frac{[Fd]}{[Fd_T]} \frac{[NADPH]}{K_2} \right)}{K_{mNADP} \left(1 + \frac{[NADP^+]}{K_{mNADP}} + \frac{[NADPH]}{K_{mNADPH}} \right)} \dots\dots (44)$$

$$v_{cet} = V_{2M} [Q_{ib}] [Fd_r] / [Fd_T] \dots\dots (44)$$

$$Q_H = \frac{H_{f1}}{H_{f1} + 10^{-pK}} \dots\dots (45)$$

$$CA = 1 \dots\dots (46)$$

$$CB = K_{rae3} + \frac{K_{rae2} K_{rae3}}{[C]} + [Eaf] - [MT] \dots\dots (47)$$

$$CC = - [MT] \left(K_{rae3} + \frac{K_{rae2} K_{rae3}}{[C]} \right) \dots\dots (48)$$

$$[Mg^{2+}_s] = \frac{-CB + \sqrt{CB^2 - 4CA \cdot CC}}{2CA} \dots\dots (49)$$

$$[EC] = \frac{[Eaf]}{1 + \frac{K_{rae2}}{[C]} + \frac{[Mg^{2+}_s]}{K_{rae3}}} \dots\dots (50)$$

$$[E] = \frac{[EC] K_{rae2}}{[C]} \dots\dots (51)$$

$$[ECM] = \frac{[EC] [Mg^{2+}_s]}{K_{rae3}} \dots\dots (52)$$

$$k_{ra} = [\text{activase}] / 13014 \dots\dots (53)$$

$$v_{ra1} = k_{ra} [ER] \max \{ (1 - [ADP] / (3[ATP])), 0 \} \dots\dots (54)$$

$$v_{ra7} = k_{ra7} [ECM] [RuBP] \dots \dots (55)$$

$$v_{ran7} = k_{ran7} [ECMR] \dots \dots (56)$$

$$v_{ra6_1} = \frac{k_{ra6} [ECMR] [C]}{([C] + k_c (1 + \frac{[O]}{k_o}))} \dots \dots (57)$$

$$v_{ra6_2} = \frac{[k_{ra6}/3] [ECMR] [O]}{([O] + k_o (1 + \frac{[C]}{k_c}))} \dots \dots (58)$$

$$v_{av} = [Ax] k_{av} \dots \dots (59)$$

$$v_{va} = [Vx] k_{av} pHReg \dots \dots (60)$$

$$v_{az} = [Ax] k_{av} pHReg \dots \dots (61)$$

$$v_{za} = [Zx] k_{za} \dots \dots (62)$$

$$pHReg = 1 \dots \dots (pH_1 \leq 5.8) \dots \dots (63)$$

$$pHReg = \frac{6.5 - pH_1}{0.7} \dots \dots (6.5 > pH_1 \geq 5.8) \dots \dots (64)$$

$$pHReg = 0 \dots \dots (pH_1 > 6.5) \dots \dots (65)$$

$$Xstate = \frac{[Zx]}{[Ax] + [Vx] + [Zx]} \dots \dots (66)$$

$$k_{dm} = k_{dm0} \max\{Xstate/0.3, 1\} \dots \dots (67)$$

$$k_r = k_{r0} \max\{Xstate/0.3, 1\} \dots \dots (68)$$

$$v_{e2PRK} = k_{e2PRK} ([Thio_r] [PRK_o] - \frac{[Thio_o] [PRK_r]}{KE_{2PRK}}) \dots \dots (69)$$

$$v_{e2GADPH} = k_{e2GADPH} \left([\text{Thio}_r] [\text{GADPH}_o] - \frac{[\text{Thio}_o] [\text{GADPH}_r]}{\text{KE}_{2GADPH}} \right) \dots \dots (70)$$

$$v_{e2FBPase} = k_{e2FBPase} \left([\text{Thio}_r] [\text{FBPase}_o] - \frac{[\text{Thio}_o] [\text{FBPase}_r]}{\text{KE}_{2FBPase}} \right) \dots \dots (71)$$

$$v_{e2SBPase} = k_{e2SBPase} \left([\text{Thio}_r] [\text{SBPase}_o] - \frac{[\text{Thio}_o] [\text{SBPase}_r]}{\text{KE}_{2SBPase}} \right) \dots \dots (72)$$

$$v_{e2ATPase} = k_{e2ATPase} \left([\text{Thio}_r] [\text{ATPase}_o] - \frac{[\text{Thio}_o] [\text{ATPase}_r]}{\text{KE}_{2ATPase}} \right) \dots \dots (73)$$

$$v_{e2RuACT} = k_{e2RuACT} \left([\text{Thio}_r] [\text{Activase}_o] - \frac{[\text{Thio}_o] [\text{Activase}_r]}{\text{KE}_{2RuACT}} \right) \dots \dots (74)$$

$$v_{e2ATPGPP} = k_{e2ATPGPP} \left([\text{Thio}_r] [\text{ATPGPP}_o] - \frac{[\text{Thio}_o] [\text{ATPGPP}_r]}{\text{KE}_{2ATPGPP}} \right) \dots \dots (75)$$

$$v_{eFd2Thio} = k_{eFd2Thio} \left([\text{Fd}_r] [\text{Thio}_o] - \frac{[\text{Thio}_r] [\text{Fd}_o]}{\text{KE}_{\text{Fd2Thio}}} \right) \dots \dots (76)$$

Section 1.2 *Differential equations used in the model* Similar to the rate equations described above, only the additional differential equations pertinent to the excitation energy and electron transfer processes around PSI, the modified Q cycle, nonphotochemical quenching, ion transfer between lumen and stroma, ATP and NADPH synthesis, and regulatory mechanisms are listed here.

$$\frac{d[\text{ISPH}_{\text{red}}]}{dt} = v_{\text{bf2}} - v_{\text{bf8}} \dots \dots (1)$$

$$\frac{d[\text{Cytf}]}{dt} = v_{\text{bf9}} - v_{\text{bf8}} \dots \dots (2)$$

$$\frac{d[\text{ISP}_{\text{ox}}]}{dt} = v_{\text{bf8}} - v_{\text{bf1}} \dots \dots (3)$$

$$\frac{d[\text{ISP}_{\text{ox}}\text{PQH}_2]}{dt} = v_{\text{bf1}} - v_{\text{bf2}} \dots \dots (4)$$

$$\frac{d[\text{PQH}^-]}{dt} = v_{\text{bf}2} - v_{\text{bf}3} \dots \dots \dots (5)$$

$$\frac{d[\text{Cytb}_L]}{dt} = v_{\text{bf}4} - v_{\text{bf}3} \dots \dots \dots (6)$$

$$\frac{d[\text{PQ}_{\text{ib}}]}{dt} = v_{\text{bf}7} - v_{\text{bf}5} - v_{\text{cet}} \dots \dots \dots (7)$$

$$\frac{d[\text{PQ}]}{dt} = v_{\text{bf}3} - v_{\text{bf}7} - 0.5v_{\text{qb}} \dots \dots \dots (8)$$

$$\frac{d[\text{Cytb}_H]}{dt} = v_{\text{bf}6} - v_{\text{bf}4} + v_{\text{bf}5} \dots \dots \dots (9)$$

$$\frac{d[\text{PQ}^-]}{dt} = v_{\text{bf}5} - v_{\text{bf}6} + v_{\text{cet}} \dots \dots \dots (10)$$

$$\frac{d[\text{PQ}^{2-}]}{dt} = v_{\text{bf}6} - 0.5v_{\text{qi}} \dots \dots \dots (11)$$

$$\frac{d[\text{PQH}_2]}{dt} = 0.5v_{\text{qi}} - v_{\text{bf}1} + 0.5v_{\text{qb}} \dots \dots \dots (12)$$

$$\frac{d[\text{PC}]}{dt} = v_{\text{bf}10} - v_{\text{bf}9} \dots \dots \dots (13)$$

$$\frac{d[\text{P}_{700}]}{dt} = v_{\text{bf}10} - v_{\text{bf}15} \dots \dots \dots (14)$$

$$\frac{d[\text{K}_s^+]}{dt} = v_{\text{bf}12} \dots \dots \dots (15)$$

$$\frac{d[\text{Mg}_s^{2+}]}{dt} = v_{\text{bf}13} \dots \dots \dots (16)$$

$$\frac{d[\text{Cl}_s^-]}{dt} = v_{\text{bf}14} \dots \dots \dots (17)$$

$$\frac{d[\text{A}_{\text{ip}}]}{dt} = v_{\text{icp}} + v_{\text{inp}} - v_{\text{ipc}} - v_{\text{dp}} - v_{\text{fp}} \dots \dots \dots (18)$$

$$\frac{d[\text{U}_i]}{dt} = v_{\text{ipc}} + v_{\text{inc}} - v_{\text{icp}} - v_{\text{dc}} - v_{\text{fc}} \dots \dots \dots (19)$$

$$\frac{d[\text{A}_0^-]}{dt} = v_{\text{bf}15} - v_{\text{bf}16} \dots \dots \dots (20)$$

$$\frac{d[\text{Fd}_r]}{dt} = v_{\text{bf}16} - 27v_{\text{bf}n2} \dots \dots \dots (21)$$

$$\frac{d[\text{BFH}_s + \text{H}_s^+]}{dt} = 4v_{\text{bf11}} - \frac{v_{\text{qb}}}{27} - \frac{v_{\text{qi}}}{27} - v_{\text{bfn2}} \dots \dots (22)$$

$$\frac{d[\text{BFH}_1 + \text{H}_1^+]}{dt} = \frac{v_{\text{bf8}}}{27} + \frac{v_{\text{bf3}}}{27} + \frac{4v_{\text{s3s0}}}{27} - 4v_{\text{bf11}} \dots \dots (23)$$

$$\frac{d(\text{pH}_s)}{dt} = -0.001 (4v_{\text{bf11}} - \frac{v_{\text{qb}}}{27} - \frac{v_{\text{qi}}}{27} - v_{\text{bfn2}}) / K_{\text{bs}} \dots \dots (24)$$

$$\frac{d(\text{pH}_1)}{dt} = -0.001 (\frac{v_{\text{bf8}}}{27} + \frac{v_{\text{bf3}}}{27} + \frac{4v_{\text{s3s0}}}{27} - 4v_{\text{bf11}}) / K_{\text{b1}} \dots \dots (25)$$

$$\frac{d(k_d)}{dt} = k_r (Q_{\text{H}} d_{\text{max}} - k_d) \dots \dots (26)$$

$$\frac{d[\text{ATP}]}{dt} = v_{\text{bf11}} - v_2 - v_{23} - v_{13} - v_{113} \dots \dots (27)$$

$$\frac{d[\text{ER}]}{dt} = v_{\text{ran1}} - v_{\text{ra1}} \dots \dots (28)$$

$$\frac{d[\text{Eaf}]}{dt} = v_{\text{ra1}} - v_{\text{ra7}} + v_{\text{ran7}} + v_{\text{ra6}_1} + v_{\text{ra6}_2} - v_{\text{ran1}} \dots \dots (29)$$

$$\frac{d[\text{ECMR}]}{dt} = v_{\text{ra7}} - v_{\text{ran7}} - v_{\text{ra6}_1} - v_{\text{ra6}_2} \dots \dots (30)$$

$$\frac{d[\text{RuBP}]}{dt} = v_{\text{ra1}} - v_{\text{ra7}} + v_{\text{ran7}} + v_{13} - v_{\text{ran1}} \dots \dots (31)$$

$$\frac{d[\text{PGCA}]}{dt} = v_{\text{ra6}_2} - v_{112} \dots \dots (32)$$

$$\frac{d[V_x]}{dt} = v_{\text{av}} - v_{\text{va}} \dots \dots (33)$$

$$\frac{d[A_x]}{dt} = v_{\text{va}} - v_{\text{av}} + v_{\text{za}} - v_{\text{az}} \dots \dots (34)$$

$$\frac{d[Z_x]}{dt} = v_{\text{az}} - v_{\text{za}} \dots \dots (35)$$

$$\frac{d[\text{GADPH}_r]}{dt} = v_{\text{e2GADPH}} \dots \dots (36)$$

$$\frac{d[\text{FBPase}_r]}{dt} = v_{\text{e2FBPase}} \dots \dots (37)$$

$$\frac{d[\text{SBPase}_r]}{dt} = v_{e2\text{SBPase}} \dots \dots (38)$$

$$\frac{d[\text{PRK}_r]}{dt} = v_{e2\text{PRK}} \dots \dots (39)$$

$$\frac{d[\text{ATPase}_r]}{dt} = v_{e2\text{ATPase}} \dots \dots (40)$$

$$\frac{d[\text{ADPGPP}_r]}{dt} = v_{e2\text{ADPGPP}} \dots \dots (41)$$

$$\frac{d[\text{Activase}_r]}{dt} = v_{e2\text{RuAct}} \dots \dots (42)$$

$$\frac{d[\text{Thio}_r]}{dt} = v_{e\text{Fd2Thio}} - v_{e2\text{GAPDH}} - v_{e2\text{FBPase}} - v_{e2\text{SBPase}} - v_{e2\text{PRK}} - v_{e2\text{ATPGPP}} - v_{e2\text{RuACT}} \dots \dots (43)$$

$$\frac{d[\text{Fd}_r]}{dt} = \frac{v_{\text{bf16}}}{27} - v_{e\text{Fd2Thio}} - v_{\text{bfn2}} \dots \dots (44)$$

Section 2.1 The rate equations of C3 photosynthetic carbon metabolism model (Zhu et al. 2007). The subscripts of $v_1, v_2 \dots v_{131}$ correspond to the numbers in Fig. 1. The kinetic parameters in the rate equations are listed in Appendices B. See Appendix A for definitions of abbreviations.

$$v_1 = \frac{[\text{RuBP}]W_c \cdot \min(1, \frac{[\text{RuBP}]}{[E_t]})}{([\text{RuBP}] + K_r(1 + \frac{[\text{PGA}]}{K_{I11}} + \frac{[\text{FBP}]}{K_{I12}} + \frac{[\text{SBP}]}{K_{I13}} + \frac{[\text{Pi}]}{K_{I14}} + \frac{[\text{NADPH}]}{K_{I15}}))} \dots \dots \dots (1)$$

$$W_c = \frac{V_{Cmax}[\text{CO}_2]}{[\text{CO}_2] + K_{M11}(1 + \frac{[\text{O}_2]}{K_{M12}})} \dots \dots \dots (2)$$

$$v_2 = \frac{V_2([\text{PGA}][\text{ATP}] - \frac{[\text{DPGA}][\text{ADP}]}{K_{E2}})}{([\text{PGA}] + K_{M21})([\text{ATP}] + K_{M22}(1 + \frac{[\text{ADP}]}{K_{M23}}))} \dots \dots \dots (3)$$

$$v_3 = \frac{V_3[\text{DPGA}][\text{NADPH}]}{([\text{DPGA}] + K_{M31})([\text{NADPH}] + K_{M32})} \dots \dots \dots (4)$$

$$v_5 = \frac{V_5([\text{GAP}][\text{DHAP}] - \frac{[\text{FBP}]}{K_{E5}})}{K_{M51}K_{M52}(1 + \frac{[\text{GAP}]}{K_{M51}} + \frac{[\text{DHAP}]}{K_{M52}} + \frac{[\text{FBP}]}{K_{M53}} + \frac{[\text{GAP}][\text{DHAP}]}{K_{M51}K_{M52}})} \dots \dots \dots (5)$$

$$v_6 = \frac{V_6 \left([\text{FBP}] - \frac{[\text{F6P}][\text{Pi}]}{K_{E6}} \right)}{[\text{FBP}] + K_{M61} \left(1 + \frac{[\text{F6P}]}{K_{I61}} + \frac{[\text{Pi}]}{K_{I62}} \right)} \dots\dots\dots (6)$$

$$\text{TEMP1} = [\text{Xu5P}] \left(1 + \frac{[\text{E4P}][\text{Ri5P}]}{K_{m71}} \right) + [\text{E4P}] + [\text{Ri5P}] \dots\dots\dots (7)$$

$$\text{Den} = 1 + \left(1 + \frac{[\text{GAP}]}{K_{M72}} \right) \left(\frac{[\text{F6P}]}{K_{M104}} + \frac{[\text{S7P}]}{K_{M103}} \right) + \frac{[\text{GAP}]}{K_{M102}} + \frac{\text{TEMP1}}{K_{M101}} \dots\dots\dots (8)$$

$$v_7 = \frac{V_7 ([\text{F6P}][\text{GAP}]K_{E7} - [\text{Xu5P}][\text{E4P}])}{(K_{M71}K_{M101}\text{Den})} \dots\dots\dots (9)$$

$$v_8 = \frac{V_8 \left([\text{DHAP}][\text{E4P}] - \frac{[\text{SBP}]}{K_{E8}} \right)}{([\text{E4P}] + K_{M82}) ([\text{DHAP}] + K_{M81})} \dots\dots\dots (10)$$

$$v_9 = \frac{V_9 \left([\text{SBP}] - \frac{[\text{Pi}][\text{S7P}]}{K_{E9}} \right)}{[\text{SBP}] + K_{M9} \left(1 + \frac{[\text{Pi}]}{K_{I9}} \right)} \dots\dots\dots (11)$$

$$v_{10} = \frac{V_{10} ([\text{GAP}][\text{S7P}]K_{E10} - [\text{Ri5P}][\text{Xu5P}])}{(K_{M71}K_{M101}\text{Den})} \dots\dots\dots (12)$$

$$v_{13} = \frac{V_{13} Y [\text{ATP}][\text{Ru5P}] - [\text{ADP}][\text{RuBP}] Y}{Y [\text{ATP}] Y 1 + \frac{[\text{ADP}]}{K_{I134}} Y + K_{M132} \left(1 + \frac{[\text{ADP}]}{K_{I135}} \right) Y \left([\text{Ru5P}] + K_{M131} \left(1 + \frac{[\text{PGA}]}{K_{I131}} + \frac{[\text{RuBP}]}{K_{I132}} + \frac{[\text{Pi}]}{K_{I133}} \right) \right)}$$

..... (13)

$$v_{16} = \frac{V_{16} Y [\text{ADP}][\text{Pi}] - \frac{[\text{ATP}] Y}{K_{E13}}}{K_{M161} K_{M162} Y 1 + \frac{[\text{ADP}]}{K_{M161}} + \frac{[\text{Pi}]}{K_{M162}} + \frac{[\text{ATP}]}{K_{M163}} + \frac{[\text{ADP}]}{K_{M161}} \frac{[\text{Pi}]}{K_{M162}} Y}$$

▣ EMBED Equation.3 ▣▣▣

$$1 + \frac{[\text{ATP}]}{K_{M232}} + \frac{[\text{G1P}]}{K_{M231}} + \frac{[\text{ATP}][\text{G1P}]}{K_{M232} K_{M231}} + \frac{[\text{ADPG}]}{K_{M233}} + \frac{[\text{OPOP}]}{K_{M234}} + \frac{[\text{ADPG}][\text{OPOP}]}{K_{M233} K_{M234}} + \frac{[\text{Pi}]}{K_{I23}}$$

..... (15)

$$v_{24} = \frac{V_{24} [\text{ADPG}]}{K_{M241} + [\text{ADPG}]}$$

▣ EMBED Equation.3 ▣▣▣

$$v_{25} = V_{25} Y 1 - \frac{[\text{RuBP}]}{5} Y \frac{[\text{ATP}]}{Y [\text{ATP}] + 1 Y}$$

▣ EMBED Equation.3 ▣▣▣

$$N = 1 + (1 + \frac{K_{M313}}{[P_{ext}]}) (\frac{[Pi]}{K_{M312}} + \frac{[PGA]}{K_{M32}} + \frac{[GAP]}{K_{M33}} + \frac{[DHAP]}{K_{M311}}) \dots \dots \dots (18)$$

$$v_{31} = \frac{V_{31}[DHAP]}{K_{M311}N} \dots \dots \dots (19)$$

$$v_{32} = \frac{V_{32}[PGA]}{K_{M32}N} \dots \dots \dots (20)$$

$$v_{33} = \frac{V_{33}[GAP]}{K_{M33}N} \dots \dots \dots (21)$$

$$v_{51} = \frac{V_{51} Y [GAPc] [DHAPc] - \frac{[FBPc]_Y}{K_{E51}}}{K_{m512} \times K_{m513} Y 1 + \frac{[GAPc]}{K_{m512}} + \frac{[DHAPc]}{K_{m513}} + \frac{[FBPc]}{K_{m513}} + \frac{[GAPc] [DHAPc]_Y}{K_{m512} K_{m513}}} \quad \text{EMBED Equation.3}$$

$$v_{52} = \frac{V_{52} Y [FBPc] - \frac{[F6Pc][Pic]_Y}{K_{E52}}}{K_{m521} \times Y 1 + \frac{[F26BPc]_Y Y 1}{K_{I523}} + \frac{[FBPc]}{K_{m521} \times Y 1 + \frac{[F26BPc]_Y}{K_{I523}}} + \frac{[Pic]}{K_{I522}} + \frac{[F6Pc]}{K_{I521}} + \frac{[Pic] [F6Pc]_Y}{K_{I522} K_{I521}}} \quad \text{EM}$$

$$v_{55} = \frac{V_{55} ([UTPc] [G1Pc] - \frac{[UDPGc] [OPOPc]}{K_{E551}})}{K_{m551} K_{m552} (1 + \frac{[UTPc]}{K_{m551}} + \frac{[G1Pc]}{K_{m552}} + \frac{[UDPGc]}{K_{m553}} + \frac{[OPOPc]}{K_{m554}} + \frac{[UTPc] [G1Pc]}{K_{m551} K_{m552}} + \frac{[UDPGc] [OPOPc]}{K_{m553} K_{m554}})}$$

..... (24)

$$v_{56} = \frac{V_{56} ([F6Pc] [UDPGc] - \frac{[SUCPc] [UDPc]}{K_{E56}}) (\frac{2 [HexPc]}{[HexPc] + 2})}{([F6Pc] + K_{m561} (1 + \frac{[FBPc]}{K_{I562}})) ([UDPGc] + K_{m562} (1 + \frac{[UDPc]}{K_{I561}})) (1 + \frac{[SUCPc]}{K_{I563}}) (1 + \frac{[SUCc]}{K_{I565}}) (1 + \frac{[Pic]}{K_{I564}})}$$

..... (25)

$$v_{57} = \frac{V_{57} ([SUCPc] - \frac{[SUCc] [Pic]}{K_{E57}})}{[SUCPc] + K_{m571} (1 + \frac{[SUCc]}{K_{I572}})} \dots \dots \dots (26)$$

$$v_{58} = \frac{V_{58} [F26BPc]}{Y [F26BPc] + K_{M581} Y 1 + \frac{[F6Pc]_Y Y 1}{K_{I581}} + \frac{[FBPc]_Y Y 1}{0} + \frac{[Pic]_Y Y 1}{K_{I582}} + \frac{[F6Pc]_Y}{K_{I583}}} \quad \text{EMBED Equation.3}$$

$$v_{59} = \frac{V_{59} Y[\text{ATPc}][\text{F6Pc}] - \frac{[\text{ADPc}][\text{F26BPc}]_Y}{K_{E59}}}{Y[\text{F6Pc}] + K_{m593} Y \left([\text{ATPc}] + K_{m591} Y 1 + \frac{[\text{ADPc}]_Y}{K_{I591}} \right)} \quad \text{EMBED Equation.3}$$

$$v_{60} = \frac{V_{60}([\text{ATPc}][\text{UDPc}] - [\text{ADPc}][\text{UTPc}]/K_{E60})}{K_{m602}K_{m603} \left(1 + \frac{[\text{ATPc}]}{K_{m602}} + \frac{[\text{UDPc}]}{K_{m603}} + \frac{[\text{ATPc}][\text{UDPc}]}{K_{m602} \times K_{m603}} + \frac{[\text{ADPc}]}{K_{m601}} + \frac{[\text{UTPc}]}{K_{m604}} + \frac{[\text{ADPc}][\text{UTPc}]}{K_{m601}K_{m604}} \right)}$$

..... (29)

$$v_{111} = \frac{W_o[\text{RuBP}] \min \left(1, \frac{[\text{RuBP}]}{[E_t]} \right)}{\left([\text{RuBP}] + K_r \left(1 + \frac{[\text{PGA}]}{K_{I11}} + \frac{[\text{FBP}]}{K_{I12}} + \frac{[\text{SBP}]}{K_{I13}} + \frac{[\text{Pi}]}{K_{I14}} + \frac{[\text{NADPH}]}{K_{I15}} \right) \right)} \quad \text{..... (30)}$$

$$W_o = \frac{V_{111}[\text{O}_2]}{[\text{O}_2] + K_o \left(1 + \frac{[\text{CO}_2]}{k_C} \right)} \quad \text{..... (31)}$$

$$v_{112} = \frac{V_{112}[\text{PGCA}]}{[\text{PGCA}] + K_{m112} \left(1 + \frac{[\text{GCA}]}{K_{i1121}} \right) \left(1 + \frac{[\text{Pi}]}{K_{I1122}} \right)} \quad \text{..... (32)}$$

$$v_{113} = \frac{V_{113} \left([\text{ATP}][\text{GCEA}] - \frac{[\text{ADP}][\text{PGA}]}{K_{E113}} \right)}{\left([\text{ATP}] + K_{m1131} \left(1 + \frac{[\text{PGA}]}{K_{i113}} \right) \right) \left([\text{GCEA}] + K_{m1132} \right)} \quad \text{..... (33)}$$

$$v_{121} = \frac{V_{121}[\text{GCAc}]}{[\text{GCAc}] + K_{m121}} \quad \text{..... (34)}$$

$$v_{122} = \frac{V_{122} \left([\text{GOAc}][\text{SERc}] - \frac{[\text{HPRc}][\text{GLYc}]}{K_{E122}} \right)}{\left([\text{GOAc}] + K_{m1221} \right) \left([\text{SERc}] + K_{m1222} \left(1 + \frac{[\text{GLYc}]}{K_{i1221}} \right) \right)} \quad \text{..... (35)}$$

$$v_{1in} = V_{1T} \frac{[GCEAc]}{[GCEAc] + K_{M1011} \left(1 + \frac{[GCAc]}{K_{I1011}}\right)} \dots\dots (36)$$

$$v_{1out} = V_{1T} \frac{[GCEA]}{[GCEA] + K_{M1011} \left(1 + \frac{[GCA]}{K_{I1011}}\right)} \dots\dots (37)$$

$$v_{2out} = V_{2T} \frac{[GCA]}{[GCA] + K_{M1012} \left(1 + \frac{[GCEA]}{K_{I1012}}\right)} \dots\dots (38)$$

$$v_{2in} = V_{2T} \frac{[GCAc]}{[GCAc] + K_{M1012} \left(1 + \frac{[GCEAc]}{K_{I1012}}\right)} \dots\dots (39)$$

$$[T3P] = [GAP] + [DHAP]. \dots\dots (40)$$

$$[Pent] = [Ru5P] + [Ri5P] + [Xu5P]. \dots\dots (41)$$

$$[HexP] = [G6P] + [F6P] + [G1P]. \dots\dots (42)$$

$$[GAP] = \frac{[T3P]}{1 + K_{e4}} \dots\dots (43)$$

$$[DHAP] = \frac{K_{e3}[T3P]}{1 + K_{e4}} \dots\dots (44)$$

$$[Ru5P] = \frac{[Pent]}{\frac{1}{K_{E11}} + \frac{1}{K_{E12}} + 1} \dots\dots (45)$$

$$[Ri5P] = \frac{\frac{1}{K_{E11}} [Pent]}{\frac{1}{K_{E11}} + \frac{1}{K_{E12}} + 1} \dots\dots (46)$$

$$[Xu5P] = \frac{\frac{1}{K_{E12}} [Pent]}{\frac{1}{K_{E11}} + \frac{1}{K_{E12}} + 1} \dots\dots (47)$$

$$[G6P] = \frac{[HexP]}{\frac{1}{K_{E21}} + K_{E22} + 1} \dots\dots (48)$$

$$[F6P] = \frac{\frac{1}{K_{E21}} [HexP]}{\frac{1}{K_{E21}} + K_{E22} + 1} \dots\dots (49)$$

$$[G1P] = \frac{K_{E22}[HexP]}{\frac{1}{K_{E21}} + K_{E22} + 1} \dots\dots (50)$$

$$[CA] = [ADP] + [ATP]. \dots (51)$$

$$[CN] = [NADP] + [NADPH]. \dots (52)$$

$$[CP] = [Pi] + [PGA] + 2[BPGA] + [GAP] + [DHAP] + 2[FBP] + [F6P] + [E4P] + 2[SBP] + [S7P] + [Xu5P] + [Ri5P] + [Ru5P] + 2[RuBP] + [G6P] + [G1P] + [ATP] + [PGCA]. \dots (53)$$

$$[CA_c] = [ADP_c] + [ATP_c]. \dots (54)$$

$$[CP_c] = 2 * ([FBP_c] + [F26BP_c]) + [PGA_c] + [T3P_c] + [HexP_c] + [SUCP] + [UTP_c] + [ATP_c] + [Pi]. \dots (55)$$

$$[CN_c] = [NAD_c] + [NADH_c]. \dots (56)$$

$$[CU_c] = [UDP_c] + [UTP_c]. \dots (57)$$

Section 2.2 Differential equations to describe rates of change in each intermediate of

carbon metabolism (Zhu et al. 2007).. See Appendix A for definition of v_1, v_2

..... v_{131} .

$$\frac{d[RuBP]}{dt} = v_{13} - v_1 - v_{111} \dots (1)$$

$$\frac{d[PGA]}{dt} = 2v_1 - v_2 - v_{32} + v_{111} + v_{113} \dots (2)$$

$$\frac{d[DPGA]}{dt} = v_2 - v_3 \dots (3)$$

$$\frac{d[T3P]}{dt} = v_3 - 2v_5 - v_7 - v_8 - v_{10} - v_{31} - v_{33} \dots (4)$$

$$\frac{d[FBP]}{dt} = v_5 - v_6 \dots (5)$$

$$\frac{d[E4P]}{dt} = v_7 - v_8 \dots (6)$$

$$\frac{d[S7P]}{dt} = v_9 - v_{10} \dots (7)$$

$$\frac{d[SBP]}{dt} = v_8 - v_9 \dots (8)$$

$$\frac{d[ATP]}{dt} = v_{16} - v_2 - v_{23} - v_{13} - v_{113} - v_{25} \dots (9)$$

$$\frac{d[HexP]}{dt} = v_6 - v_7 - v_{23} + v_{25} \dots (10)$$

$$\frac{d[PenP]}{dt} = v_7 + 2v_{10} - v_{13} \dots (11)$$

$$\frac{d[\text{GOAc}]}{dt} = v_{121} - v_{122} - v_{124} \dots \dots \dots (12)$$

$$\frac{d[\text{SER c}]}{dt} = v_{131} - v_{122} \dots \dots \dots (13)$$

$$\frac{d[\text{GLY c}]}{dt} = v_{122} + v_{124} - 2v_{131} \dots \dots \dots (14)$$

$$\frac{d[\text{HPRc}]}{dt} = v_{122} - v_{123} \dots \dots \dots (15)$$

$$\frac{d[\text{GCEAc}]}{dt} = v_{123} - v_{1in} + v_{1out} \dots \dots \dots (16)$$

$$\frac{d[\text{GCEA}]}{dt} = v_{1in} - v_{113} - v_{1out} \dots \dots \dots (17)$$

$$\frac{d[\text{GCA}]}{dt} = v_{112} - v_{2out} + v_{2in} \dots \dots \dots (18)$$

$$\frac{d[\text{PGCA}]}{dt} = v_{111} - v_{112} \dots \dots \dots (19)$$

$$\frac{d[\text{GCAc}]}{dt} = v_{2out} - v_{121} - v_{2in} \dots \dots \dots (20)$$

$$\frac{d[\text{OPOPc}]}{dt} = v_{55} - v_{61} \dots \dots \dots (21)$$

$$\frac{d[\text{UTPc}]}{dt} = v_{60} - v_{55} \dots \dots \dots (22)$$

$$\frac{d[\text{SUCPc}]}{dt} = v_{56} - v_{57} \dots \dots \dots (23)$$

$$\frac{d[\text{SUCc}]}{dt} = v_{57} - v_{62} \dots \dots \dots (24)$$

$$\frac{d[\text{PGAc}]}{dt} = v_{32} - v_{\text{pga_use}} \dots \dots \dots (25)$$

$$\frac{d(\text{T3Pc})}{dt} = v_{31} + v_{33} - 2v_{51} \dots \dots \dots (26)$$

$$\frac{d(\text{FBPc})}{dt} = v_{51} - v_{52} \dots \dots \dots (27)$$

$$\frac{d[\text{HexPc}]}{dt} = v_{52} - v_{55} - v_{59} + v_{58} - v_{56} \dots \dots \dots (28)$$

$$\frac{d[\text{F26BPc}]}{dt} = v_{59} - v_{58} \dots \dots \dots (29)$$

$$\frac{d[\text{UDPGc}]}{dt} = v_{55} - v_{56} \dots \dots \dots (30)$$

$$\frac{d[\text{ATPc}]}{dt} = v_{\text{atpf}} - v_{59} - v_{60} \dots \dots \dots (31)$$