



# From leaf to multiscale models of photosynthesis: applications and challenges for crop improvement

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Received: 26 January 2024 / Accepted: 29 January 2024  
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## Abstract

To keep up with the growth of human population and to circumvent deleterious effects of global climate change, it is essential to enhance crop yield to achieve higher production. Here we review mathematical models of oxygenic photosynthesis that are extensively used, and discuss in depth a subset that accounts for diverse approaches providing solutions to our objective. These include models (1) to study different ways to enhance photosynthesis, such as fine-tuning antenna size, photoprotection and electron transport; (2) to bioengineer carbon metabolism; and (3) to evaluate the interactions between the process of photosynthesis and the seasonal crop dynamics, or those that have included statistical whole-genome prediction methods to quantify the impact of photosynthesis traits on the improvement of crop yield. We conclude by emphasizing that the results obtained in these studies clearly demonstrate that mathematical modelling is a key tool to examine different approaches to improve photosynthesis for better productivity, while effective multiscale crop models, especially those that also include remote sensing data, are indispensable to verify different strategies to obtain maximized crop yields.

**Keywords** C4 rice · Improving photosynthesis and crop yield · Leaf and crop models · Photorespiration bypasses · Photosynthesis models · Synthetic biology

## Abbreviations

$C_i$ ,  $C_m$ ,  $C_c$  Intercellular, mesophyll, or chloroplast  $\text{CO}_2$  concentration  
CAM Crassulacean acid metabolism, a pathway of  $\text{CO}_2$  assimilation

CBB cycle	Calvin-Benson-Bassham cycle of $\text{CO}_2$ assimilation
CCM	$\text{CO}_2$ concentrating mechanism
CET	Cyclic electron transport
Chl	Chlorophyll
Cyt	Cytochrome
$\Delta\Psi$	Electric potential difference across the thylakoid membrane
$\Delta\text{pH}$	pH difference across the thylakoid membrane
ETR	Electron transport rate
Fe-S	Rieske iron sulfur protein, an electron carrier
Fd	Ferredoxin, an electron carrier
FNR	Ferredoxin-NADP <sup>+</sup> oxidoreductase
LHCI, LHCII	Light-harvesting complexes in PSI and PSII antenna
NADP <sup>+</sup>	Oxidized form of nicotinamide adenine dinucleotide phosphate, an electron carrier
NDH	NADH dehydrogenase-like complex involved in antimycin A insensitive cyclic electron transport

This is a review dedicated to the memory of Kenneth (Ken) Sauer (1931–2022), a friend of one of us (Govindjee).

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NPQ	Nonphotochemical quenching of the excited state of chlorophyll
OEC	Oxygen evolving complex of PSII
P680, P700	The primary electron donor of PSII and of PSI, respectively
PGR5/PGR1	A complex containing Proton Gradient Regulation 5 and Proton Gradient Regulation Like 1 proteins involved in antimycin A sensitive cyclic electron transport
<i>pmf</i>	Proton motive force
$P_N$	The net photosynthetic rate
PQ and PQH <sub>2</sub>	Plastoquinone and its reduced form, plastoquinol
PSI, PSII	Photosystem I and II
PTOX	Plastid terminal oxidase, involved in chlororespiration
Q <sub>A</sub> , Q <sub>B</sub>	First and second plastoquinone electron acceptors of PSII
Rac	Rubisco activase
ROS	Reactive oxygen species
Rubisco	Ribulose-1,5-bisphosphate carboxylase/oxygenase
SIF	Solar induced fluorescence
TM	Thylakoid membrane
WWC	Water-water cycle

## Introduction: improving the efficiency of photosynthesis for a better crop yield

In oxygenic photosynthesis, plants capture light energy from the sun and produce sugars and organic biomass from CO<sub>2</sub> and water, releasing molecular oxygen into the atmosphere as a byproduct (Blankenship 2021; Björn et al. 2023). This process has had a fundamental role in shaping the history of Earth, by contributing to the rise of atmospheric O<sub>2</sub> and the evolution of animals (Sánchez-Baracaldo and Cardona 2020). It was and is the source of our food, fiber, biofuel, and many other useful substances. As the human population is expected to reach 10.87 billion by 2100, much more primary foodstuff would be needed to feed us all. It has been estimated that the production of the current major field crops such as wheat, rice, maize, and soybean, which provide about two thirds of calories consumed globally, must double by 2050 (see e.g., Long and Ort 2010; Long et al. 2015). Since a corresponding expansion of the available cultivable land is not sustainable (Muhie 2022), it is necessary to find ways to increase the crop yields. Moreover, the ongoing climate change has diminished the crop productivity in the last 25 years, which also highlights the necessity of having higher crop yields in the future (Long 2012; Ray et al. 2012, 2013; Arora 2019). Yet, the progress in disease protection and fertilization, as well as the classical breeding measures

taken to improve production during the green revolution in the late twentieth century (such as dwarfing; see Peng et al. 1999; Parry et al. 2011), cannot continue at present to lead alone to sufficient advancement in the crop yield (Evans and Fischer 1999; Sinclair et al. 2004; Sharma-Natu and Ghildiya 2005; Long et al. 2015; Furbank et al. 2020).

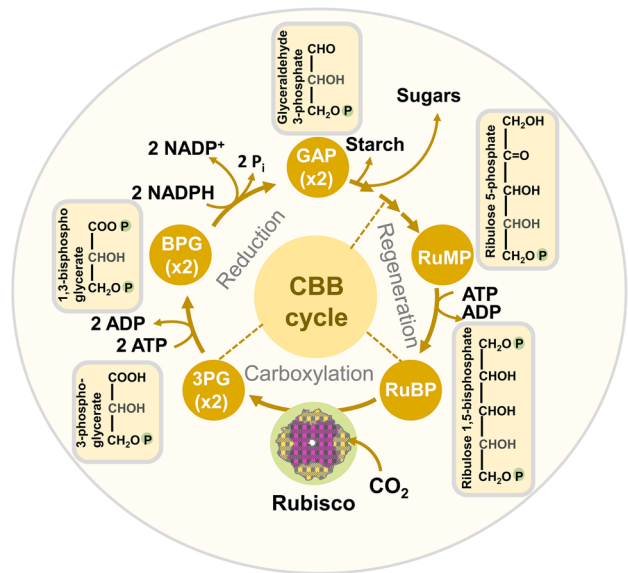
Furthermore, theoretical considerations show that the efficiency ( $\epsilon$ ) of light conversion to biomass is  $\sim 0.03$  at the best in plants, which is only one-third of the theoretical maximum of  $\sim 0.09$ , while under the field conditions it is even lower (Zhu et al. 2004a, 2008, 2010). Since improvement in photosynthesis (i.e., with a higher  $\epsilon$ ) was not addressed during the green revolution (Gifford and Evans 1981; Koester et al. 2016), the enhancement of photosynthesis is now considered an important target to increase crop productivity, as any increases in the net photosynthesis rate of individual plants may lead to increases in biomass across the entire growing season and crop canopy (Long et al. 2006; Zhu et al. 2010; Evans 2013; Long 2014; Ort et al. 2015). Experimental evidence supporting this point of view has been obtained in field experiments using the *free-air* CO<sub>2</sub> enrichment (FACE) method, in which higher biomass and yield was achieved in plants grown under elevated CO<sub>2</sub> (Ainsworth et al. 2004; Long et al. 2006; Kang et al. 2021; Ainsworth and Long 2021), as well as in studies in which the rate of photosynthesis was enhanced through genetic engineering (e.g., Kromdijk et al. 2016; Köhler et al. 2017; Lopez-Calcano et al. 2020; De Souza et al. 2022). A variety of possible ways to improve photosynthesis have been suggested and reviewed, in which both advanced non-transgenic phenomics approaches and transgenic technologies are expected to play a major role (e.g., Long et al. 2006, 2015; Ort et al. 2015; Yin and Struik 2015; Foyer et al. 2017; Dann and Leister 2017; Wu et al. 2019; Muhie 2022; Zhu et al. 2010, 2022; Walter and Kromdijk 2022; Yin et al. 2022). These include: (i) enhancing light capture; (ii) optimizing the photosynthetic electron transport to increase NADPH and ATP production; (iii) optimizing the photoprotection mechanisms; (iv) increasing photosynthesis induction under fluctuating light; (v) reducing photorespiration losses; (vi) boosting the enzymatic activity in the Calvin-Benson-Bassham (CBB) cycle; (vii) improving the flow of CO<sub>2</sub> through the leaf, or introducing CO<sub>2</sub> concentrating mechanisms around Rubisco from algae and cyanobacteria in C3 plants; (viii) optimizing the resource investment among the components of the photosynthetic apparatus to maximize carbon gain; and (ix) engineering C4 or intermediary pathways in C3 grain crops, such as rice or wheat. Together, the above modifications are expected to double the yield potential of the major crops (Zhu et al. 2010). Although there are encouraging results from some of the above methods, in a number of model species under field conditions (see e.g., Kromdijk et al. 2016; South et al. 2019; Cavanagh et al. 2022), other methods

(e.g., viii and ix) are long term projects. We emphasize that many of the above options to enhance plant productivity require modelling to guide the necessary changes via in-silico-assisted bioengineering (Long et al. 2015), or to provide information on the genes that would enhance crop photosynthesis (Yin et al. 2022). In view of the above, we highlight, in this review, several significant modelling studies aiming to find solutions for crop yield improvement and include the importance of solar-induced fluorescence (SIF) measurements towards this goal. We begin by providing an overview on the basics of photosynthesis and on modeling oxygenic photosynthesis with the goal of improving plant productivity.

## Basic information on oxygenic photosynthesis and its modelling

### Oxygenic photosynthesis: a background

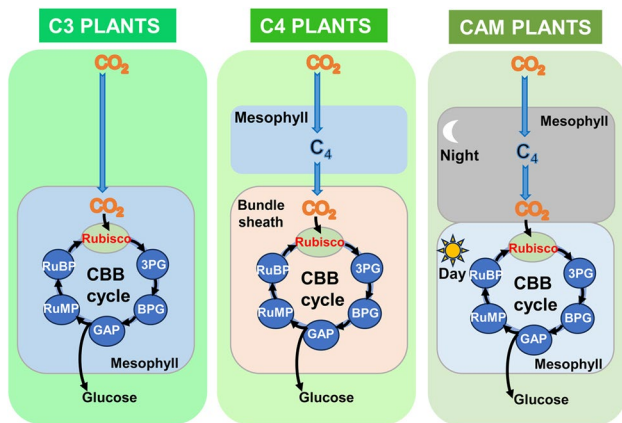
It is well known that oxygenic photosynthesis is one of the most studied biological processes (Blankenship and Govindjee 2007; Braun 2020; Stirbet et al. 2020; Shevela et al. 2019, 2023), providing a great advantage for its modelling. During the initial light phase, taking place in the thylakoids (the specialized membrane system in the chloroplast), light energy is harvested by both photosystem (PS) I and PSII antenna, and transferred to their respective reaction centers, where photochemical reactions take place (Sauer 1975, 1979; Mirkovic et al. 2017). This process initiates electron transfer from water to  $\text{NADP}^+$  in a linear chain of electron carriers (Pushkar et al. 2008; Govindjee et al. 2017), leading as well to cyclic and pseudo cyclic electron transport, in addition to the formation of NADPH and ATP, the major event. In the second phase of oxygenic photosynthesis in C3 species, taking place in the chloroplast stroma, the Calvin-Benson-Bassham (CBB) cycle, the C3 cycle, is the central part of the overall carbon metabolism (Fig. 1), which uses the reducing power of NADPH and the energy from ATP, both produced by the light reactions, to do the job. The CBB cycle involves 11 enzymes that catalyze 13 reactions, where ribulose 1,5-bisphosphate carboxylase/oxygenase (Rubisco) is the key enzyme (for its discovery, see Sharkey 2023). It is involved in the fixation of  $\text{CO}_2$  (carboxylation) on ribulose 1,5-bisphosphate (RuBP), a five-carbon compound producing two molecules of 3-phosphoglycerate (3PG), which are used for biosynthetic reactions and the recycling of RuBP (Fig. 1). The necessary light activation of this process is achieved by covalent redox-modification of some key enzymes that are inactive in the dark. For a historical background of the CBB cycle, see Calvin (1989), Benson (2002), Bassham (2003), Nonomura et al. (2017),



**Fig. 1** A diagram of the Calvin–Benson–Bassham (CBB) cycle for carbon assimilation ( $\text{CO}_2$  fixation) in oxygenic photosynthesis. The three stages of the CBB cycle are: (i) *Carboxylation* the enzyme Rubisco catalyzes the incorporation of  $\text{CO}_2$  into RuBP (ribulose 1,5-bisphosphate), a molecule with five carbon atoms, resulting in the formation of two molecules of 3-phosphoglycerate (3PG), each with three atoms of carbon; (ii) *Reduction* NADPH (together with ATP) are used to reduce the 3PG molecules to glyceraldehyde 3-phosphate (GAP), which is used for the biosynthesis of starch and sugars; and (3) *Regeneration* ribulose bis phosphate (RuBP), the molecule that starts the cycle, is regenerated, in several steps, by using ATP, so that the cycle can continue. Modified from Shevela and Govindjee (2016)

Sharkey (2019), and for mathematical models of the C3 photosynthesis see e.g., Farquhar et al. (1980), Poolman et al. (2000), Laisk et al. (2006), Zhu et al. (2007, 2013), Jablonsky et al. (2011), Morales et al. (2018a, b) and Belasio (2019).

We emphasize here that Rubisco is not very discriminating with respect to  $\text{CO}_2$  and  $\text{O}_2$  (see e.g., Farquhar et al. 1980; Zhu et al. 2008), since it also catalyzes, as a side-reaction, the fixation of molecular  $\text{O}_2$  on RuBP, which leads to the formation of one molecule of 3-phosphoglycerate (3PG), and one molecule of 2-phosphoglycolate (2PG). The 2PG is then converted to glycolate (Ogren and Bowes 1971; Bauwe 2023), which can inhibit at least three enzymes of the CBB cycle, and, thus, it must be quickly removed. The glycolate is detoxified through a complex photorespiration cycle, also known as the C2 cycle (Hodges et al. 2016; Busch 2020), involving reactions taking place in chloroplasts, mitochondria, peroxisomes, and the cytosol. The rate of photorespiration depends on the reaction kinetics of Rubisco and the atmospheric conditions: the oxygenation decreases as the  $[\text{CO}_2]$  increases, and the specificity of Rubisco for  $\text{CO}_2$  relative to  $\text{O}_2$  decreases as the temperatures increase, thus increasing



**Fig. 2** Schematic illustration of C3, C4, and the crassulacean acid metabolism (CAM) pathways of photosynthesis in plants. *C<sub>4</sub>*, malate, a four-carbon compound that releases CO<sub>2</sub> after decarboxylation; *CBB cycle*, Calvin-Benson-Bassham cycle of carbon assimilation (see Fig. 1); *Rubisco*, ribulose-1,5-bisphosphate carboxylase/oxygenase; *3PG*, 3-phosphoglycerate; *BPG*, 1,3-bisphosphoglycerate; *GAP*, glyceraldehyde 3-phosphate; *RuMP*, ribulose 5-phosphate; *RuBP*, ribulose 1,5-bisphosphate. Modified from <https://ib.bioninja.com.au/higher-level/topic-8-metabolism-cell/untitled-2/c3-c4-and-cam-plants.html>

the rates of oxygenation. Due to photorespiration, 75% of the carbon in 2PG is recycled, and can reenter the C3 cycle, but the efficiency of C3 photosynthesis decreases significantly, since the photorespiration requires additional ATP and NADPH (Walker et al. 2016).

Although the C3 pathway for carbon assimilation in plants is predominant on Earth, there are plants which use other metabolic pathways (Fig. 2): (i) C4, also known as the Hatch-Slack pathway (Hatch and Slack 1966); and (ii) the crassulacean acid metabolism (CAM). Note that C4 and CAM pathways are adaptations that have evolved independently multiple times over the past 30 million years (see e.g., Sage et al. 2012; Schlüter and Weber 2020).

The C4 pathway leads to increased [CO<sub>2</sub>] at Rubisco, counteracting the effect of oxygen, and enhancing the carbon assimilation efficiency, which, together with improved nitrogen and water use efficiencies, leads to higher biomass production in several crops, such as sugarcane, sorghum, and maize. To achieve the above, C4 plants have developed a special anatomy (the so-called Kranz anatomy; e.g., Hatch and Osmond 1976; Fouracre 2014), where mesophyll and bundle sheath cells have different structures and functions (see Fig. 2). However, after 2000, C4 photosynthesis was shown to occur also in single mesophyll cells of a few plant species, due to their unique intracellular compartmentalization, equivalent to that between mesophyll and bundle sheath cells in the Kranz anatomy (see reviews by Edwards et al. 2004; Sharpe and Offermann 2014). The C4 photosynthesis starts in the mesophyll cells, where the CO<sub>2</sub> is

converted into bicarbonate by carbonic anhydrase, and then the latter is ‘fixed’ on phosphoenolpyruvate (PEP, a three-carbon compound) by PEP carboxylase (PEPC), producing oxaloacetate (OAA, a four-carbon compound), which is then converted into malate (also a four-carbon compound) by malate dehydrogenase. Then, the malate is transported to the bundle sheath cells, where it is decarboxylated to release CO<sub>2</sub>, which is used by the CBB cycle in the chloroplasts of the bundle sheath cells. The remaining pyruvate is translocated back to the mesophyll cells and reconverted to PEP, using ATP. For mathematical models of C4 photosynthesis see e.g., Laisk and Edwards (2000), von Caemmerer and Furbank (2003), Zhu et al. (2008), Bellasio (2016), Wang et al. (2014a,b; 2021), von Caemmerer (2021). Based on the enzymes used to decarboxylate the C4 acids in the bundle sheath cells, the C4 plants are of the following subtypes: (i) NADP-malic enzyme (ME) (e.g., in: maize, sorghum, sugarcane, and millet); (ii) NAD-ME (e.g., in: *Atriplex rosea*, *Panicum milioides*, and *Portulaca oleracea*); and (iii) phosphoenolpyruvate carboxykinase (PEP-CK) (e.g., in the guinea grass *Megathyrus maximus*). However, by using a modelling analysis, Wang et al. (2014a) have concluded that only the NADP-ME and NAD-ME should be considered separate C4 subtypes, as they both intrinsically involve a supplementary PEP-CK cycle. On the other hand, the optimal energetic requirements of 80% energy allocation in the bundle sheath cells and 20% in the mesophyll cells, which was determined in their theoretical analysis, cannot be fulfilled in a pure PEP-CK type plant, because, in the Kranz anatomy, the bundle sheath cells are shaded by the mesophyll cells.

Further, the CAM pathway is a special metabolism used by plants, such as the succulent ones that grow in extremely arid environments. These plants separate the photosynthetic function in time, in order to conserve water and fix CO<sub>2</sub> at high concentrations, without photorespiration (Winter and Smith 2022). This is done in the following manner (see Fig. 2): (i) when the stomata are open at night (i.e., when it is cooler), CO<sub>2</sub> is fixed on PEP, using PEP carboxylase, and the resulting oxaloacetate is converted to malate, which is stored in the vacuoles of the mesophyll cells; and (ii) when the stomata are closed during the day (i.e., when the temperature is high), the malate from the vacuoles is transported into the mesophyll chloroplasts and, there, it is decarboxylated releasing CO<sub>2</sub> which then feeds into the CBB cycle, while the remaining pyruvate is converted back to PEP. For models of CAM photosynthesis, see e.g., Cheung et al. (2014) and a review by Burgos et al. (2022).

## Background on mathematical modelling of oxygenic photosynthesis

Models of oxygenic photosynthesis can be classified into empirical, mechanistic, quasi-mechanistic, as well as steady-state or dynamic, depending on the assumptions made, their formulation, and applications. There is a great deal of diversity among the models as they describe the entire photosynthetic process in different ways, but they can be also incomplete, depicting either the light or the carbon reactions (or parts of these), depending on the research question raised, as well as the available data. The very early models related to carbon assimilation were *empirical* (e.g., Maskell 1928), being based on the relationship between the net photosynthesis rate ( $P_N$ ) and the environmental variables such as light intensity ( $I$ ), temperature ( $T$ ), and  $\text{CO}_2$  concentration ( $C_i$  or  $C_c$ , i.e., the intercellular  $\text{CO}_2$  concentration, or that in chloroplasts). This method has been used by many researchers, with numerous variations, and consists of an algebraic function containing several parameters, which is relatively simple and easy to use to fit the experimental data, but without the description of the physiological processes of photosynthesis (see e.g., Smith 1936; Jassby and Platt 1976; Eilers and Peeters 1988; Ye 2007). However, when such an empirical model is combined with a steady-state mechanistic model of photosynthesis, which links biochemical properties of the leaves to gas exchange measurements (see e.g., Farquhar et al. 1980), the newer unified model can indeed provide information on key photosynthetic parameters ‘capturing’ the underlying physiological processes of photosynthesis. For different protocols, proposed for fitting the dependence of photosynthesis or the electron transport rate ( $ETR$ , noted also as flux  $J$ ) on environmental variables by using such a combined model, see e.g. (1) Ögren and Evans (1993), von Caemmerer (2000), Johnson and Murchie (2011), Ye et al. (2013a,b; 2020; 2024), and Herrmann et al. (2020) for net photosynthesis-light response curves, ( $P_N/I$ ) and ( $J/I$ ); (2) Long and Bernacchi (2003), Sharkey et al. (2007), Dubois et al. 2007, Miao et al. (2009), and Gu et al. (2010) for net photosynthesis-intercellular  $\text{CO}_2$  response curves ( $P_N/C_i$ ); and (3) Medlyn et al. (2002), Hikosaka et al. (2006) and Adams et al. (2017) for net photosynthesis-temperature response curves ( $P_N/T$ ). We note that the  $P_N/I$  curves are characteristic for the photosynthetic phenotype of plants, and a combined model (as those mentioned above) gives information on the quantum yield, the maximum photosynthetic capacity, the leaf radiation use efficiency, and the light compensation point (Johnson and Murchie 2011). The  $P_N/C_i$  curves, as determined from gas exchange measurements, have been successfully used to evaluate the parameters defined by the Farquhar et al. (1980) model, or its variants (Yin et al. 2009). Since these models are commonly used to estimate the  $\text{CO}_2$  assimilation from the leaf to the global

scale (Yin and Struik 2009; Bernacchi et al. 2013; Rogers et al. 2017; Wu et al. 2016, 2019), quantitative evaluation of their parameters is necessary for the estimation of crop and ecosystem productivity, and together with the results obtained from the  $P_N/T$  curves, they are essential for the evaluation of climate change impact on the entire system (von Caemmerer 2013, 2021).

However, the *mechanistic photosynthetic models* (steady-state or dynamic) are based on biochemical and biophysical principles that describe the reactions and pathways of photosynthesis. Although they are more realistic and explanatory, they require many more parameters as well as data to be calibrated and validated (see e.g., Antal et al. 2013). *Mechanistic steady-state models*, as those just described above, assume that the photosynthetic reactions are in equilibrium, i.e., the concentrations of intermediates do not change over time, and thus they consist of a set of algebraic equations containing parameters characterizing the photosynthetic system. The steady-state model of C3 photosynthesis, proposed by Graham Farquhar, Susanne von Caemmerer and Joseph Berry (Farquhar et al. 1980), often referred to as the FvCB model, is one of the most widely used models in plant science. This model consists of a small number of algebraic equations describing the steady-state  $\text{CO}_2$  exchange in C3 leaves—that relates the biochemistry of  $\text{CO}_2$  assimilation to gas exchange—and accounts for the limitations imposed by Rubisco activity, electron transport capacity, and  $\text{CO}_2$  diffusion, within the leaf. The FvCB model has now many improved variants with additions such as: (1) temperature dependence of  $\text{CO}_2$  assimilation from the chloroplast to the ecosystem level (Bernacchi et al. 2001, 2002, 2013), and the mesophyll conductance process (Moore et al. 2021); (2) adjustments for C4 photosynthesis (von Caemmerer and Furbank 2003; Wang et al. 2014a,b; von Caemmerer 2021), or for C3–C4 photosynthesis (von Caemmerer 2000; Bellassio 2016); (3) inclusion of alternative electron transport pathways (Yin et al. 2004); (4) generalization of a mesophyll resistance model for different intracellular arrangements of chloroplasts and mitochondria (Yin and Struik 2017); and (5) inclusion of possible effects of cyanobacterial bicarbonate transporters at the chloroplast envelope (Price et al. 2011). The above-cited steady-state models of photosynthesis are simple, easy to use for the analysis of experimental data, and for the exploration of different ways to improve photosynthesis, such as optimizing the distribution of resources between different enzymes of the carbon metabolism, redirecting photorespiratory  $\text{CO}_2$  to implement bicarbonate pumps in C3 chloroplasts, or to insert C4, CAM or intermediate C3–C4 forms of photosynthesis into C3 plants, and for exploring potential benefits of engineering different photosynthetic traits into crops (for additional applications, see reviews by von Caemmerer 2000, 2013; Yin et al. 2021).

When investigating the response of photosynthesis to rapid variations of different environmental variables, *mechanistic dynamic models* are much more appropriate than the steady-state photosynthesis model, since the photosynthetic processes in this case are continuously adjusted to match the various changes of the environment (Kaiser et al. 2015). Dynamic models are usually based on the use of ordinary differential equation systems describing the kinetics of the reactions involved in photosynthesis, such as electron transport and carbon fixation, but they can be also based on stochastic or probabilistic methods, or contain related elements.

Many available models of photosynthesis have focused on the kinetics of the underlying processes related to the induction of photosynthesis during transition from the dark to the light, such as Chl fluorescence induction; for the relation between the Chl fluorescence and photosynthesis, see Papageorgiou and Govindjee (2004), Kalaji et al. (2016, 2017, 2018), Brestic and Allakhverdiev (2022), and Stirbet et al. (2019). There are models of Chl fluorescence induction that do not consider the carbon assimilation reactions (e.g., Stirbet and Strasser 1996; Stirbet et al. 1998; Lazár 2003, 2009, 2013; Tomek et al. 2003; Sušila et al. 2004; Lazár et al. 2005a; Zhu et al. 2005; Guo and Tan 2011, 2014; Ebenhöf et al. 2014; Belyaeva et al. 2019; Riznichenko and Rubin 2021), or those which include both the light and carbon assimilation reactions and other related metabolic reactions (e.g., Laisk et al. 2006, 2009a; Zhu et al. 2013); see reviews by Stirbet et al. (2014, 2020), and a book on photosynthesis in silico (Laisk et al. 2009b). On the other hand, minimized models of photosynthesis have been used by Morales et al. (2018a) and Bellasio (2019) to analyze the photosynthetic electron transport regulation and to simulate experimental data measured with different methods, or by Fu et al. (2020) to verify a feedback control framework for regulating photosynthetic activities. The effects of natural fluctuating light on the rate of photosynthesis have been also analyzed (see e.g., Way and Percy 2012; Morales et al. 2018b; Slattery et al. 2018); for reviews, see Morales and Kaiser 2020; Long et al. 2022), as well as artificial fluctuating light (e.g., Lazár et al. 2022a). In the latter case, multiple factors influence the rate of photosynthesis, such as changes in stomatal and mesophyll conductance, NPQ relaxation, Rubisco activation/de-activation, activation of RuBP regeneration enzymes, and metabolite pool sizes; further, the relative importance of these factors varies with the species of the plant or of the algae (e.g., Taylor and Long 2017; De Souza et al. 2022). On the other hand, simultaneous changes of several other environmental factors (e.g., variations in leaf temperature, leaf-to-air vapor pressure deficit  $VPD_{\text{leaf-air}}$ , and atmospheric  $[CO_2]$ ) also induce perturbations in plants (Kaiser et al. 2017), which cause e.g., changes in  $C_i$  (Peak and Mott 2011), and thus in the rate of carbon assimilation and the crop yield (Taylor and Long 2017; Wang et al. 2021).

Furthermore, dynamic models of photosynthesis have been used to verify hypotheses regarding spontaneous oscillations in photosynthesis (e.g., Laisk and Walker 1986; Laisk et al. 1991; Lazár et al. 2005b; see a review by Walker 1992), and to calculate the flux control coefficient (CC) of enzymes for  $CO_2$  uptake rate (Poolman et al. 2000), as well as to identify targets to enhance photosynthesis (Poolman 1999; Zhu et al. 2007; Wang et al. 2021; see also Zhu et al. 2010). In addition, we note that for the quantitative understanding of complex metabolic pathways, related to carbon assimilation reactions, with the goal of altering the distribution of metabolic flux or of designing metabolic pathways for new products, mathematical modelling of metabolism is definitely an important tool (Giersch 2000).

Finally, different multiscale crop models, having at their base available models of photosynthesis, are currently being developed, and these will be mentioned in the last section of this review: Crop models are imperative to improve crop yield.

### Fine-tuning the light phase of photosynthesis to obtain a greater crop yield

Several reviews have recently been published on how to optimize/improve the light-dependent photosynthetic reactions to increase plant productivity (see e.g., Cardona et al. 2018; Murchie and Ruban 2020; Sukhova et al. 2021; Walter and Kromdijk 2022; Leister 2023; Wu et al. 2023). For this goal, the following aspects of the light-phase of photosynthesis need to be considered (see the blue stars in Fig. 3). The quality (i.e., the wavelengths) of the light absorbed by the photosystems has been shown to strongly influence the efficiency of photosynthesis (see e.g., Hamdani et al. 2019a; and a review by Lazár et al. 2022b). Moreover, since PSII and PSI work in series, any imbalance in their relative excitations will affect negatively on the photosynthetic process; however, there is regulation and re-equilibration through a complex process known as the ‘*state-transition*’, in which a part of the PSII antenna (a mobile LHCII complex) is relocated from PSII to PSI, or the other way around, as a function of the redox state of the plastoquinone (PQ) pool (see e.g., Papageorgiou and Govindjee 2011; see blue star 1 in Fig. 3). Moreover, if the light already absorbed by PSII is in excess, the excited state can be quenched non-photochemically as heat (Demmig et al. 1987; Jahns and Holzwarth 2012; Papageorgiou and Govindjee 2014; see blue star 2 in Fig. 3). If the absorbed light is still in excess, it leads to the formation of reactive oxygen species (ROS), which can be, however, scavenged, in a complicated manner, by the water-water cycle (WWC; see Foyer 2018 and blue star 5 in Fig. 3). An important feature of photosynthetic electron transport in the

thylakoid membrane (TM) during the “light phase” of photosynthesis is that it is coupled to proton transport across the membrane, leading to acidification of the lumen (see e.g., Buchanan 1980). The low lumen pH, thus formed, not only initiates the NPQ, but it is also a part of the proton motive force ( $pmf$ ) driving ATP synthesis (Mitchell 1975); in addition, it causes photosynthesis control at the level of Cyt  $b_6/f$  (Wilson et al. 2021; Trinh and Masuda 2022; see blue star 3 in Fig. 3). Cyclic electron transport (CET) around PSI (see blue star 4 in Fig. 3) also contributes to acidification of lumen (e.g., Kawashima et al. 2017). As the other part of  $pmf$  is the electric potential difference, caused by redistribution of ions between the two sides of the TM, i.e., the membrane potential,  $\Delta\Psi$  (see blue star 6 in Fig. 3), it is important to consider the partitioning of  $pmf$  into  $\Delta\Psi$  and  $\Delta pH$  (see blue star 7 in Fig. 3). All the processes, namely the state transitions, the NPQ, the water-water cycle, the photosynthesis control, and the membrane potential have been mathematically modelled as described below.

### The state transitions

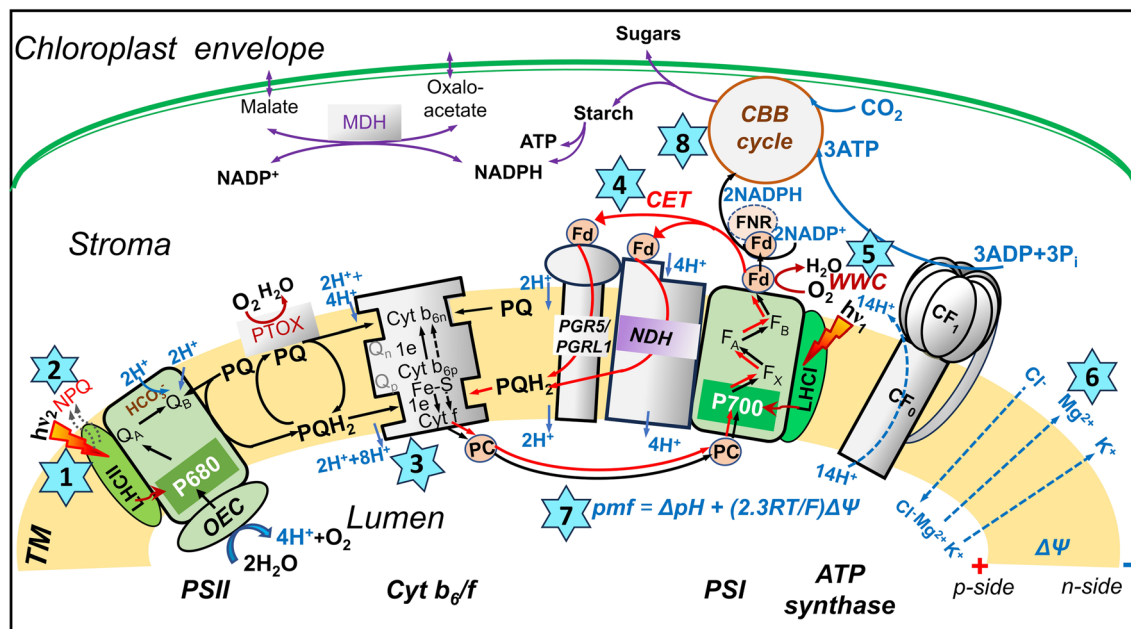
As mentioned earlier, the state transitions take place to provide a balanced excitation between the two photosystems (Allen et al. 1981). PQ pool reduction by the PSII under excess light leads to the activation of a kinase (STN7 in plants; Stt7 in algae) that phosphorylates a fraction of the LHCII in the PSII antenna, which, in accord with the most popular view of this process (see a review by Rochaix 2014), moves in the TM towards PSI, and attaches to its antenna. In this way, a transition from the high fluorescence State 1 to the low fluorescence State 2 takes place, since PSI has lower fluorescence yield than PSII. If this is followed by exposure to low light, the PQ pool is oxidized by the higher light absorption of PSI, which then inactivates the kinases, and the constitutively active PHP1/TAP38 phosphatase dephosphorylates the mobile LHCII complexes from PSI antenna, which then move back to PSII, leading to a State 2 to State 1 transition. Fine tuning of the state transitions and of the rates of their adjustment/accommodation in fluctuating light might lead to a better light management and thus, potentially to higher plant productivity. Indeed, Negi et al. (2020) have bioengineered a mutant of *C. reinhardtii* which dynamically adjusts the size of its light harvesting antenna as a function of the growth light intensity; this mutant shows higher photosynthetic rates, and two to three-fold greater biomass productivity, while preserving the ability to induce state transitions and nonphotochemical quenching (NPQ) of the excited state of Chl  $a$  (Demmig et al. 1987; see Fig. 3).

The state transitions have been mathematically modelled by Ebenhöf et al. (2014), and an essentially similar model was used by Stirbet and Govindjee (2016) for the same phenomenon. In both cases, the modelling involved

the state transitions in the green alga *Chlamydomonas reinhardtii*, grown under low light, when the NPQ is only slightly involved. Ebenhöf et al. (2014) assessed the state-transition by using Pulse Amplitude Modulation (PAM) fluorescence measurements and simulations of changes in the maximal ChlF ( $F_M'$ ) under very low as well as high light. On the other hand, Stirbet and Govindjee (2016) used Chl  $a$  fluorescence induction measurements under continuous illumination and confirmed in silico that under anaerobic conditions in the darkness, the PQ pool is reduced by chlororespiration using PTOX (the plastid terminal oxidase; see Fig. 3), which triggers a State 1 to State 2 transition. In the subsequent in silico illumination under aerobic conditions, a State 2 to State 1 transition occurs, causing a slow Chl  $a$  fluorescence rise from the S-step to a maximum M in the simulated slow Chl fluorescence induction curve [Note that the “step S” follows the usual OJIP phase of the Chl  $a$  fluorescence transient, where P to S is a fluorescence decline due mostly to the ferredoxin-NADP<sup>+</sup> oxidoreductase (FNR) activation and NPQ induction by lumen acidification, see e.g., Briantais et al. 1979]. Additionally, Stirbet and Govindjee (2016) analyzed, also in silico, how light intensity and different photosynthetic processes influence the degree of state transitions, and thus the relative amplitude of the simulated S-M increase.

### The non-photochemical quenching of the excited state of chlorophyll $a$

Similar to the state transition, a faster induction of the NPQ under excess light and a faster relaxation of NPQ under low light, might be a way for the plants and algae to better manage the light and thus to increase plant productivity. The so-called fast NPQ (denoted as  $qE$ ) is triggered by acidification of the lumen, which causes protonation of the PsbS protein and the activation of violaxanthin de-epoxidase (VDE); VDE converts violaxanthin to zeaxanthin via antheraxanthin. Further, protonated PsbS, and zeaxanthin are necessary for the induction of the NPQ in excess light (Jahns and Holzwarth 2012). Under low light (or in darkness), zeaxanthin epoxidase (ZE) converts zeaxanthin back to antheraxanthin, and then to violaxanthin, causing a decrease in NPQ. Different mathematical models have been formulated by choosing different molecular aspects of NPQ (for reviews, see Zaks et al. 2013; Bennett et al. 2018; Morris and Fleming 2018). D’Haese et al. (2004), however, focused specifically on the role of VDE and the conversion of violaxanthin to antheraxanthin and zeaxanthin. On the other hand, Ebenhöf et al. (2011) presented a more detailed model of NPQ, based on zeaxanthin being converted by VDE, which is activated by acidification of the lumen. And this was then improved by Zaks et al. (2012) and Matuszyńska et al. (2016) by the inclusion of protonated PsbS for having a more complete



**Fig. 3** Schematic representation of the ‘light phase’ of oxygenic photosynthesis in plants. Several protein complexes in the thylakoid membranes (TM) of the chloroplast participate in the production of ATP and NADPH needed for the CBB cycle to fix CO<sub>2</sub>: PSII and PSI operating in series, Cyt *b*<sub>6</sub>/*f* complex, PGR5/PGRL1 complex, NDH, PTOX, and CF<sub>0</sub>-CF<sub>1</sub> ATP-synthase. The light energy harvested by LHCII and LHCI complexes is, respectively, channeled to P680 in PSII and P700 in PSI, where photochemical reactions take place, and the photogenerated electrons are then transported by several electron carriers through a linear electron transfer chain from water to NADPH (black arrows). The PGR5/PGRL1 and the chloroplast NDH complexes, the last one forming a super-complex with PSI, mediate two CET pathways around PSI shown by red arrows. Also, the water-water cycle (WWC), and the PTOX activity are indicated by dark-red arrows. In parallel with the electron transport, protons are also transported across TM by PSII, Cyt *b*<sub>6</sub>/*f*, PGR5/PGRL1 complex, NDH, and PTOX, leading to a pH difference ( $\Delta pH$ ) across the TM. Furthermore, the charge separation(s) in the PSI and PSII reaction centers, as well as different ion transport steps through TM, generate an electric potential difference ( $\Delta\Psi$ ) across TM, which together with  $\Delta pH$ , forms the proton motive force (*pmf*) that is used for ATP production at the ATP synthase. Finally, we show the CBB cycle, which works with NADPH, ATP and CO<sub>2</sub>, and few metabolic reactions in stroma, as indicated by purple arrows. Additionally, several bioengineering targets for the improvement of crop yield are marked with blue stars: (1) the antenna size; (2) the NPQ that develops in PSII antenna; (3) the photosynthesis control exerted by Cyt *b*<sub>6</sub>/*f*; (4) the influence of CET on  $\Delta pH$ , and thus on NPQ and ATP/NADPH ratio; (5) the influence of WWC on ROS concentration; (6) the influence of

ion transporters on  $\Delta\Psi$ ; (7) the partitioning of *pmf* into  $\Delta pH$  and  $\Delta\Psi$  components; and (8) the influence of different manipulations of the CBB cycle on CO<sub>2</sub> fixation efficiency, such as engineering Rubisco, *Rac*, photorespiration, and addition of CO<sub>2</sub> concentration mechanisms near Rubisco. Figure modified from Stirbet et al. (2020).  $2.3RT/F$ , a physical constant; *CBB cycle*, Calvin–Benson–Bassham cycle of carbon assimilation; *CET*, cyclic electron transport around PSI; *CF<sub>1</sub>* and *CF<sub>0</sub>*, a catalytic part, and a membrane-embedded part (containing a proton channel) of the ATP synthase; *Cyt*, cytochrome;  $\Delta\Psi$ , electric potential difference across the thylakoid membrane;  $\Delta pH$ , pH difference across the thylakoid membrane; *Fe-S*, Rieske iron sulfur protein, an electron carrier; *Fd*, ferredoxin iron sulfur protein, another electron carrier; *FNR*, ferredoxin-NADP<sup>+</sup> oxidoreductase; *LHCI* and *LHCII*, light-harvesting complexes of PSI and PSII, respectively; *NADP<sup>+</sup>*, nicotinamide adenine dinucleotide phosphate, oxidized form, which is a terminal electron carrier; *NDH*, NADH dehydrogenase-like complex that is involved in antimycin A insensitive cyclic electron transport; *NPQ*, nonphotochemical quenching of the excited state of chlorophyll; *OEC*, oxygen evolving complex of PSII; *P680*, *P700*, the primary electron donors of PSII and PSI; *PGR5/PGRL1*, a complex containing Proton Gradient Regulation 5 and Proton Gradient Regulation Like 1 proteins that is involved in the antimycin A sensitive cyclic electron transport; *pmf*, proton motive force; *PQ* and *PQH<sub>2</sub>*, plastoquinone and plastoquinol; *PSI* and *PSII*, Photosystem I and II; *PTOX*, plastid terminal oxidase; *Q<sub>A</sub>*, *Q<sub>B</sub>*, first and second plastoquinone electron acceptors of PSII; *Rac*, Rubisco activase; *ROS*, reactive oxygen species; *Rubisco*, ribulose-1,5-bisphosphate carboxylase/oxygenase; *TM*, thylakoid membrane; *WWC*, water-water cycle

view of NPQ. We note that in addition to zeaxanthin and protonated PsBs, a role of lutein was included by Leuenberger et al. (2017) in their model. On the other hand, a general model of NPQ, considering only PSII in the reduced and the oxidized state being either quenched or unquenched, without going into molecular details of the quenching, has been formulated by Snellenburg et al. (2017). A similar approach was also used in the model by Sukhova et al.

(2020). However, Bennett et al. (2018) related the extent of NPQ to the diffusion length of excitation, modelled as a random walk in the PSII pigment bed: the higher the quenching, the shorter the diffusion length.

Using only a phenomenological model of NPQ in response to the light history, X-G. Zhu et al. (2004a) theoretically predicted that the delay in the recovery of NPQ can lead up to a 30% decrease of canopy carbon uptake. These



theoretical predictions have been qualitatively confirmed, in tobacco, in field measurements (Kromdijk et al. 2016), and in soybean transformants overexpressing VDE, PsbS, and ZE (De Souza et al. 2022). It is important to note that the increased plant productivity of the transformants over the wild-types occurred only under fluctuating light conditions, which is, however, common in the field.

### On photoinhibition, and the water-water cycle

PSII is well-known to be easily photoinhibited, but it is also rapidly repaired (for a review, see Vass 2012). Photoinhibition of PSII, initiated by the oxidation of amino acids of PSII D1/D2 proteins by hydroxyl radical  $\text{HO}^\bullet$  and superoxide anion radical  $\text{O}_2^{\bullet-}$ , has been experimentally confirmed (Kale et al. 2017). On the other hand, photoinhibition of PSI is rare, and occurs only under certain specific conditions (reviewed in Sonoike 2011; Furutani et al. 2020), e.g., at low temperature (Tjus et al. 1998). Photoinhibition of PSI is usually inferred from the decrease of Pm (Terashima et al. 1994), the maximal transmittance at 820 nm, reflecting the oxidation state of P700, the primary electron donor in PSI reaction center.

However, Suorsa et al. (2012) showed clear PSI photoinhibition using *Arabidopsis pgr5* mutant under fluctuating light; they observed a large decrease in its Pm; this *pgr5* mutant lacks the PGR5 protein, which facilitates a type of CET around PSI (see Fig. 3). Lack of the CET in the mutant disables the photosynthesis control (see below), and decreases the outflow of electrons from PSI (Kono and Terashima 2016), both leading to the electron flow from PSI to oxygen and the formation of  $\text{O}_2^{\bullet-}$ , which damages PSI. The  $\text{O}_2^{\bullet-}$  undergoes enzymatic as well as non-enzymatic reactions known as the water-water cycle (WWC; see Fig. 3), leading to the formation of other reactive oxygen species (ROS), but also to a safe ROS scavenging (reviewed in Asada 1999, 2006). Since ROS also participate in signaling pathways (reviewed by Foyer and Hanke 2022), we note that we have here a fine tuning of WWC. The WWC has been mathematically modelled by Polle (2001), Valero et al. (2009, 2016), and Saadat et al. (2021); while Valero et al. (2009) have calculated steady-state fluxes through the WWC, Polle (2001) and Valero et al. (2016) have explored the dynamics of WWC function, respectively, under illumination by constant light, and under illumination by fluctuating light. On the other hand, Saadat et al. (2021) have presented the connection between the model of WWC with that of the CBB cycle; in addition, they have explored the WWC kinetics under fluctuating light.

### The photosynthesis control

Apart from the central role of the acidified lumen in triggering the fast NPQ, protons already present in the lumen cause a back pressure against the movement of other protons going to the lumen during (re)oxidation of the plastoquinol ( $\text{PQH}_2$ ) on the luminal side of Cyt *b<sub>6</sub>/f*. The back pressure of protons leads to a decrease of the rate constant of  $\text{PQH}_2$  reoxidation (Rumberg and Siggel 1969), the effect being the so-called *photosynthesis control* (Tikhonov et al. 1981).

Increased photosynthesis control, on the one hand, results in the accumulation of  $\text{P700}^+$  (i.e., the oxidized PSI primary donor), which prevents the photoinhibition of PSI (see e.g., Sejima et al. 2014) but, on the other hand, it decreases the amount of NADPH produced, which decreases  $\text{CO}_2$  assimilation, and thus plant productivity. Since the photosynthesis control requires a more acidified lumen than that needed for the triggering of the NPQ (Takizawa et al. 2007; Schansker 2022), fine tuning of photosynthesis control and NPQ, i.e., in fact of the luminal pH, is thus important for attaining high plant productivity. In relation to that, transgenic rice lines with variable content of Rieske protein in the Cyt *b<sub>6</sub>/f* complex (see Fe-S in Fig. 3) indeed show enhanced leaf photosynthesis, making Cyt *b<sub>6</sub>/f* complex a target to increase grain yield (Yamori et al. 2016).

We note that the light-induced acidification of the lumen is caused not only by the linear electron transport from water to  $\text{NADP}^+$ , but also by the CET around PSI (see Fig. 3), either via PGR5/PGRL1 protein complex, or via NDH-like complex (Kawashima et al. 2017; reviewed, e.g., in Shikanai 2016). Several models of different complexity have already been constructed; several describe the role of CET on the luminal pH and the role of photosynthesis control on the electron transport (Hope et al. 1994; Sato et al. 2014; Morales et al. 2018a; Matuszyńska et al. 2019; Vershubskii and Tikhonov 2020; Johnson and Berry 2021).

### The electric potential difference across the thylakoid membrane

To dissipate the charge of protons, accumulated in the lumen due to light-driven proton-coupled electron transport, counter ions ( $\text{K}^+$ ,  $\text{Cl}^-$ ,  $\text{Mg}^{2+}$ ; Hind et al. 1974) have been shown to move thorough the TM via related ion channels, which affect the electrical potential difference across the thylakoid membrane ( $\Delta\Psi$ ), leading to *pmf* ( $=\Delta\text{pH} + (2.3\text{RT}/F)\Delta\Psi$ ) partitioning (see Fig. 3), and, ultimately, this shows its impact on plant productivity (reviewed by e.g., Szabó and Spetea 2017). The role of counter ion fluxes and  $\Delta\Psi$  on photoprotection and photosynthetic performance have been clearly recognized, especially under fluctuating light conditions, by, e.g., Li et al. (2021); Lazár et al. (2022a); and von Bismarck et al. (2023). Mathematical models of  $\Delta\Psi$  of

different complexity are available (see e.g., van Kooten et al. 1986; Cruz et al. 2001; Lyu and Lazár 2017a, 2017b, 2022, 2023; Li et al. 2021), and they need to be further examined and related to future experimental data.

### Photosynthesis under fluctuating light

All of the processes mentioned above are, of course, important, especially under fluctuating light conditions, when their fine tuning/regulation is repeatedly required. Since the fluctuating light is more natural in the field than illumination with constant light intensity, as is mostly used in laboratory experiments, a large number of researchers are now exploring photosynthesis under fluctuating light conditions. Several models have now been formulated to describe the photosynthesis and its regulation under fluctuating light, and what is important, they have been related to plant and algal productivity (see e.g., Graham et al. 2017; Morales et al. 2018b; Steen et al. 2020; Krichen et al. 2021; Salvatori et al. 2022). For a better understanding of photosynthesis regulation at the molecular level, there is also a special interest in experiments that use illumination by light with its intensity changing as a sinus function (see: Nedbal and Březina 2002; Nedbal et al. 2003, 2005); this has now been supported not only by mathematical models, but by new experiments (Nedbal and Lazár 2021; Lazár et al. 2022a; Niu et al. 2024). By changing the period (frequency) of the sinusoidal wave, a resonance with a particular regulatory process can be established and thus the response of the regulatory processes to a particular frequency (period) of light oscillations is being revealed (Niu et al. 2023). Such an approach seems to be promising for finding frequency limits of particular regulatory processes, which can be important for obtaining higher plant productivity in the future.

### Synthetic biology approach for improving the plant carbon metabolism

Synthetic biology is a highly promising interdisciplinary field that integrates molecular biology with biochemical engineering, combined with computational methods. Its objective is to modify existing organisms, or to create artificial novel life forms for newer purposes, including the improvement of photosynthesis (South et al. 2018; Stewart et al. 2018).

As discussed above (see Background on oxygenic photosynthesis), the photorespiratory cycle is a complex and energy consuming set of reactions required to recycle the 2PG resulting from the oxygenation of RuBP by Rubisco (see reviews by Foyer et al. 2009; Walker et al. 2016), which takes place mainly in chloroplasts, peroxisomes,

and mitochondria. Further, photorespiration is known to be significant in C3 plants; it can increase considerably under warm and dry environments (Long et al. 2015). By using mathematical modelling, X.G. Zhu et al. (2008) showed that the maximal theoretical efficiency of gross photosynthesis in C3 plants decreases due to photorespiration by  $\approx 49\%$  at  $30^\circ\text{C}$  and 380 ppm  $[\text{CO}_2]$ . According to Walker et al. (2016), even a 5% reduction in photorespiration would be worth almost 540 million dollars a year in yield gain in the US Corn Belt alone! Therefore, decreasing photorespiration has been an early goal for crop yield improvement (see e.g., Long et al. 2006, 2015; Peterhansel and Maurino 2011; Evans 2013; Ort et al. 2015; Betti et al. 2016; Walker et al. 2016; Orr et al. 2017; South et al. 2018; Batista-Silva et al. 2020). However, this process also plays multiple metabolic and regulatory roles (Foyer et al. 2009; Timm et al. 2016; Bauwe 2023; Chen et al. 2023c). Thus, decreasing the efficiency of photorespiration must also lead to stability and beneficial regulation of plant metabolism (Walker et al. 2016). There are several approaches to bioengineer photorespiration that can reduce the carbon and energetic loss in C3 crops (Raines 2006; South et al. 2018), such as by (i) increasing the efficiency of Rubisco to assimilate  $\text{CO}_2$  through genetic manipulation; (ii) bioengineering new alternative metabolic pathways, i.e., photorespiration bypasses, by introducing non-native genes that are used to process the glycolate more efficiently; (iii) preventing Rubisco oxygenation reaction by enriching the  $[\text{CO}_2]$  at the Rubisco site, through the installation of pyrenoid or carboxysome structures obtained from single-celled algae or cyanobacteria, and, this together with the expression of bicarbonate transporters; and (iv) by enriching  $[\text{CO}_2]$  at the Rubisco site, by introducing C4 photosynthesis into C3 plants. Below, we briefly present some of these approaches.

### Bioengineering Rubiscos with higher rates of $\text{CO}_2$ assimilation

More than 90% of the inorganic carbon converted into biomass, in Nature, is fixed by Rubisco (ribulose-1,5-bisphosphate carboxylase/oxygenase), which represents 50% of all soluble proteins in a leaf, and it is the most abundant protein on Earth (Bar-On and Milo 2019); for reviews, see Spreitzer and Salvucci (2002), Erb and Zarzycki (2018), and Prywes et al. (2023); for historical aspects, see Portis and Parry (2007) and Sharkey (2023). This enzyme is known to limit carbon assimilation of C3 plants, due to its activity as oxygenase, and its low turnover frequency (i.e., between 1 and  $10\text{ s}^{-1}$ ; Erb and Zarzycki 2018). In order to increase crop production, different ways to improve the activity of Rubisco have been suggested (see e.g., Zhu et al. 2010; Raines 2003, 2011; Cummins et al. 2018; Paul 2021; Oh et al. 2023; Prywes et al. 2023). These include: (i) increasing the Rubisco

content within chloroplasts (Salesse-Smith et al 2018, 2020; Yoon et al. 2020); (ii) replacing the inefficient endogenous Rubisco with a better performing one (Zhu et al. 2004b; Lin et al. 2014); (iii) decreasing photorespiration by increasing Rubisco specificity for CO<sub>2</sub> relative to O<sub>2</sub> through genetic modification (Zhu and Long 2009; Lin et al. 2014; Carmo-Silva et al. 2015; Sharwood 2017); and (iv) manipulating the activation of Rubisco by Rubisco activase (Rca) (Mott and Woodrow 2000; Carmo-Silva et al. 2015; Perdomo et al. 2019; Chen et al. 2023a).

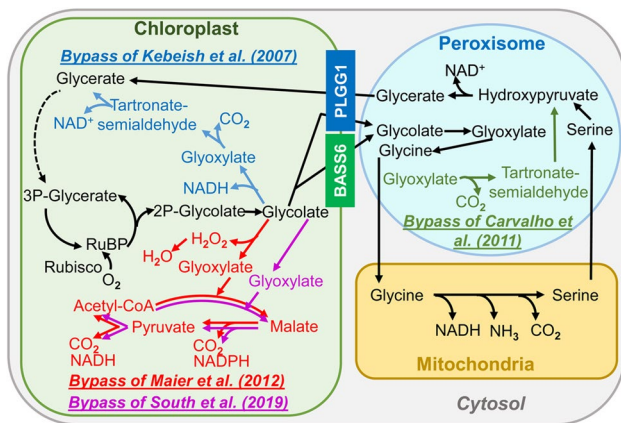
On a positive note, Salesse-Smith et al. (2018) have already obtained a > 30% increase in Rubisco content in maize by overexpressing its large (LS) and/or small (SS) subunits, as well as the Rubisco assembly chaperone RUBISCO ASSEMBLY FACTOR 1 (RAF1). The transgenic plants had 15% increased CO<sub>2</sub> assimilation (i.e., the light-saturated photosynthetic capacity, A<sub>SAT</sub>), which was correlated with higher fresh weight. The difference between the increase in Rubisco content (i.e., 30%) and that of A<sub>SAT</sub> (i.e., 15%) was accounted by a decrease in Rubisco activation state up to 23%. Furthermore, important results have been obtained also by Yoon et al. (2020), who have overexpressed Rubisco in paddy rice with its own promoter. Their study showed increases in filled spikelets, with 28% higher grain yields in paddy fields, and 11–23% higher total biomass. In addition, there was greater yield gain for nitrogen added in the transgenic rice than in the wild-type, indicating an increased nitrogen use efficiency in the former. Long (2020) suggests that this work and that of Salesse-Smith et al. (2018) “*contradict the space limitation hypothesis for C3 and C4 crops*”, which assumes that there is no physical space for a higher Rubisco content in their chloroplasts (Pyke and Leech 1987). Moreover, Long (2020) has also highlighted the results obtained by Yoon et al. (2020), stating that “*an engineered increase in photosynthetic capacity does, in fact, result in increased grain yield under production field conditions in the world’s most important cereal — rice*”.

Concerning the work on Rubisco improvement, Zhu et al. (2004b) have analyzed the potential effects on the productivity of a C3 crop plant by engineering a ‘foreign’ Rubisco with higher catalytic rates per active site (see e.g., Erb and Zarzycki 2018), and/or higher specificities for CO<sub>2</sub> relative to O<sub>2</sub>; for this, they used a steady-state biochemical model for leaf photosynthesis coupled with a canopy biophysical microclimate model. The results obtained by Zhu et al. (2004b) suggest that introducing a Rubisco with a high carboxylation rate could, indeed, lead to increased crop yields, without an increase in the amount of Rubisco per unit leaf area. Their results show that the use of Rubisco from *Amaranthus edulis* (a rare C4 plant) could increase the carbon gain by 17%, while that from *Griffithsia monilis* (a red alga) could lead to greater than 25% carbon gain. Nonetheless, the

challenges of engineering foreign Rubiscos in crop plants, or bioengineering the native ones, are still to be fully understood and exploited (Sharwood 2017; Chen et al. 2023a). Moreover, it is known that rice yields can be increased by 23%, when CO<sub>2</sub> atmospheric concentration is raised to 627 ppm (Ainsworth 2008), since the Rubisco specificity to oxygen decreases by increasing CO<sub>2</sub>. However, Hu et al. (2022) showed that to maximize this CO<sub>2</sub> fertilizer effect in the future, heat-resistant, high-yield hybrid rice cultivars with large sink capacity, and appropriate nitrogen supplement should be selected. For further information, see Cao et al. (2021).

Further, the role of Rubisco activase (Rca) on the Rubisco performance in non-steady-state photosynthesis was studied by Mott and Woodrow (2000) by using a photosynthesis model to predict the optimum protein allocation between Rubisco and Rca for plants under different light conditions, including light flecks of various duration; we note that Rca is an indispensable catalytic chaperone of Rubisco, which remodels its active site, helps the release of inhibitors, and restores its catalytic functions (Waheeda et al. 2023). Simulations by Mott and Woodrow (2000) showed that the protein distribution leading to the maximum steady-state rate of photosynthesis does not produce the maximum activation rate for Rubisco, and that in fluctuating light the plant must allocate more protein to the Rca than when exposed to constant light. Thus, further research is needed to find and improve Rubisco and Rca engineering based on the observations, mentioned above.

Finally, we note that, while Rubisco plays a key role in photosynthesis, the increased activity of other enzymes participating in the CBB cycle can also affect positively the carbon assimilation and plant growth (see e.g., Simkin et al. 2019). Indeed, modelling results have shown that the natural distribution of the enzymes within the CBB cycle is not optimal and could limit photosynthesis (Zhu et al. 2007), and that higher levels of ‘for example, sedoheptulose-1,7-bisphosphatase and fructose-1,6-bisphosphate aldolase, as well as of the enzymes related to sink capacity, could support an increased productivity (Kubis and Bar-Even 2019). For example, Morales et al. (2018a) have analyzed potential improvements in CO<sub>2</sub> assimilation resulting from optimizing different regulatory processes; their simulations showed 17% improvement when the limiting steps, related to the photo-activation of the CBB cycle enzymes and stomatal opening, were removed. Further, Matuszyńska et al. (2019) have used the metabolic control analysis (MCA) to investigate the regulatory dependence between the photosynthetic electron transport and the CBB cycle, to quantify the control distribution of ‘demand and supply’ under different light conditions; Matuszyńska and coauthors found that the ‘demand’ reactions control the flux under light-saturating conditions (with sedoheptulose-1,7-bisphosphatase maintaining the highest



**Fig. 4** Photorespiration in plants, and bioengineering approaches for its optimization. Photorespiration in C3 plants (black), with four engineered photorespiratory bypasses to increase CO<sub>2</sub> assimilation and/or reduce energy expenses; in blue is the pathway of Kebeish et al. (2007); in green is the pathway of Carvalho et al. (2011); in red is the pathway of Maier et al. (2012); and in purple is the pathway of South et al. (2019). Enzymatic reactions or metabolite transport steps are indicated by arrows. Figure modified from South et al. (2018)

overall flux control, as shown by Poolman et al. 2000), while the ‘supply’ reactions (sustained by PSII and PSI activities) show a higher overall flux control under light-limited conditions. Furthermore, Kandoi et al. (2022), who overexpressed carbonic anhydrase  $\beta$ CA3 from *Flaveria bidentis* into *Arabidopsis thaliana*, observed that this led to increased amino acid content, improved photosynthesis (by 16–22%), better water-use efficiency (by 22–26%), higher starch content (by 10–19%), and higher biomass (by 14–20%). Lastly, Hamdani et al. (2019b) discovered the importance of the  $\beta$ -glucosidase 5 gene to obtain a higher quantum yield of photosynthesis in rice—the mechanism of which remains to be further investigated.

### Reducing photorespiration by engineering synthetic bypasses routes

We now provide a glimpse of the bioengineering approach involving the introduction of alternative pathways to reduce photorespiration, i.e., the ‘photorespiratory bypasses’, such as those proposed by Carvalho (2005), Kebeish et al. (2007), Carvalho et al. (2011), and Maier et al. (2012) (also see Raines 2011; Peterhansel et al. 2013; Xin et al. 2015; Betti et al. 2016).

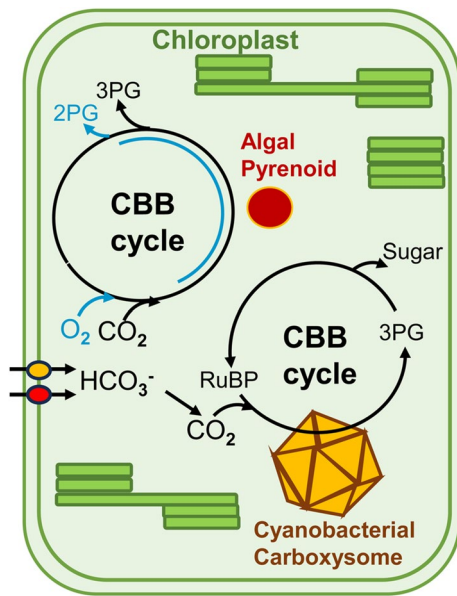
- (1) Kebeish et al. (2007) have introduced the glycolate catabolic pathway from *Escherichia coli* into *Arabidopsis thaliana*, in which the glycolate is converted to glycerate only in chloroplasts (Fig. 4, in blue), with no NH<sub>3</sub> release, but with CO<sub>2</sub> release into chloroplasts instead of mitochondria, which is energetically more

economical; it increases the net photosynthesis, as well as the biomass.

- (2) Carvalho et al. (2011; also see Carvalho 2005) engineered a photorespiratory bypass in which the glyoxylate is converted to hydroxy-pyruvate in the peroxisome (Fig. 4, in green); here, the NH<sub>3</sub> release is abolished, one-quarter of the carbon from glycolate is released as CO<sub>2</sub> in the peroxisomes, and three-quarters of the carbon from glycolate is re-converted to PG; however, the implementation of this bypass in *Nicotiana tabacum* was only partially successful.
- (3) Maier et al. (2012) introduced a photorespiration bypass in *Arabidopsis thaliana*, in which the glycolate had a complete oxidation in chloroplasts (Fig. 4, in red), with the data indicating that both the photosynthesis and biomass of the transgenic plants were enhanced.

Xin et al. (2015) have analyzed theoretically the above three bypasses by using the C3 photosynthesis model of Zhu et al. (2007), and by adding the sets of the new biochemical reactions of these bypasses. The results obtained by Xin et al. (2015) led them to the conclusion that not all photorespiration bypasses are functional or beneficial since they predict that: (i) the bypass of Kebeish et al. (2007) would increase the photosynthetic rate under a range of CO<sub>2</sub> and light conditions; (ii) the bypass of Carvalho et al. (2011) would enhance photosynthesis, but only under low light intensity; and (iii) that the bypass of Maier et al. (2012) would reduce the photosynthetic rate, which means that the loss of CO<sub>2</sub> in this pathway would not be compensated by the benefit of an increased CO<sub>2</sub> concentration in the chloroplast. However, we note that the above in silico predictions were not in complete agreement with the experimental results, as the photosynthetic rate measured by Kebeish et al. (2007) increased only under low light, and that measured by Maier et al. (2012) showed a modest increase, not a decrease. Xin et al. (2015) explained that it is difficult to predict with precision if a bypass is a viable approach to optimize the photosynthetic rate since the photorespiratory pathway can interact with many other pathways, such as the nitrogen metabolism and respiration (see also Hodges et al. 2016). However, the bypasses that increase the CO<sub>2</sub> concentration close to Rubisco in chloroplasts, and reduce the energy costs of photorespiration (by avoiding the ammonium release), are promising, and must be pursued further.

A number of other photorespiratory bypasses have been studied, and show promising results in enhancing photosynthesis in different crop plants. These include those by Nölke et al. (2014) on potato (*Solanum tuberosum*), by Dalal et al. (2015) on the biofuel crop plant *Camelina sativa*, by South et al. 2019 and Cavanagh et al. (2022) on tobacco (*Nicotiana tabacum*) (see this pathway in Fig. 4), and by Shen et al. (2019) and Wang et al. (2020) on rice (*Oryza Sativa*).



**Fig. 5** Different strategies to bioengineer carbon concentrating components in chloroplasts from C3 plants. They consist of the expression, in the chloroplast stroma, either of a functional cyanobacterial carboxysome (orange icosahedron), or an algal pyrenoid (red circle), as well as  $\text{HCO}_3^-$  transporters (red and orange ovals) on the inner chloroplast membrane. Figure modified from Batista-Silva et al. (2020). *CBB cycle*, Calvin–Benson–Bassham cycle of carbon assimilation; *2PG*, 2-phosphoglycolate; *3PG*, 3-phosphoglycerate; *RuBP*, ribulose 1,5-bisphosphate

Due to the relationship of photorespiration with other metabolic pathways (see the above discussion) adequate multi-scale crop models (see e.g., Wu et al. 2019; Wu 2023), as well as complex laboratory and field trials (see e.g., Wang et al. 2020; Cavanagh et al. 2022), are necessary for the verification of these bypasses. In view of the advances made in genome engineering and in synthetic biology, we are extremely optimistic that other possible inducible metabolic pathways will be found in the future, including those for a fully optimized photorespiration in crop plants under field conditions.

### Introducing $\text{CO}_2$ concentrating mechanisms into C3 plants

The possible effects of the addition of a cyanobacterial  $\text{CO}_2$  concentrating mechanism (i.e., a *carboxysome*; see e.g., Price et al. 2011, 2013) into a C3 crop leaf were studied theoretically by McGrath and Long (2014). We note that a carboxysome has a polyhedral structure covered with a protein shell (see Fig. 5), which contains carbonic anhydrase (CA) and Rubisco arranged in a semi-ordered array (Long et al. 2007). McGrath and Long (2014) used a kinetic model containing 9 biological compartments, as well as the photosynthesis model of Farquhar et al. (1980), to evaluate

the potential of the added carboxysome into the stroma (of the chloroplast) to improve C3 photosynthesis, and to determine the necessity of the introduction of other components, such as bicarbonate transporters. These simulations have shown that  $\approx 60\%$  improvement in the net  $\text{CO}_2$  uptake can be achieved without any modification of the leaf anatomy, and it could lead to 36%–60% increase in the crop yield; also, the addition of bicarbonate transporters is expected to further increase photosynthesis by 16%. Success in engineering  $\alpha$ -carboxisomes into tobacco chloroplasts has been obtained by Long et al. (2018), who, by using a reduced gene set, have succeeded in increasing  $\text{CO}_2$  fixation and crop yield up to 60% in a transgenic tobacco, as previously predicted by McGrath and Long (2014). Furthermore, Chen et al. (2023b) have been able to generate morphologically correct  $\alpha$ -carboxisomes, by transforming 9 carboxysome genetic components derived from a proteobacterium.

Further, we note that the modelling work of Fei et al. (2022) has provided insights into the operating principles of the pyrenoid-based  $\text{CO}_2$ -concentrating mechanism of the green alga *Chlamydomonas reinhardtii* (also see: Burlacot and Peltier 2023). Based on the results obtained with their model, as well as the data from the literature (Wang et al. 2016; Meyer et al. 2017; Mukherjee et al. 2019), Fei et al. (2022) suggest that a physical barrier is necessary for the pyrenoid to diminish the  $\text{CO}_2$  leakage, and to provide a proper localization of the enzymes to reduce the futile cycling between  $\text{CO}_2$  and bicarbonate; in addition, they have proposed a four-step path for engineering pyrenoids into crop plants. For a schematic presentation of the introduction of  $\text{CO}_2$  concentrating mechanisms into C3 plants, see Fig. 5.

### Bioengineering C4 rice

The C4 plants have a higher potential energy-conversion efficiency and improved nitrogen and water use efficiencies than the C3 plants, particularly in hot climates, due to their  $\text{CO}_2$ -concentrating mechanism at the Rubisco site in bundle sheath (BS) cells, and a reduced photorespiration (Schlüter and Weber 2020). Therefore, introducing C4 pathway into C3 plants is considered to be a highly desirable way to increase their yield (Schlüter and Weber 2016; Kubis and Bar-Even 2019). However, this is a difficult task, as key features of C4 photosynthesis must be introduced into C3 plants (Cui 2021), such as the Kranz anatomy (Hatch and Osmond 1976), which implies a spatial separation between the  $\text{CO}_2$  fixation and carbohydrate synthesis into the mesophyll (M) and BS cells. Moreover, in NADP-ME-type C4 plants, the M cells perform whole-chain electron transport, while the BS cells have low PSII activity, but high rates of CET around PSI to drive ATP synthesis, because most of NADPH is supplied by the M cells, via the malate shuttle (Munekage and Taniguchi 2017; Sales et al. 2021), which is not the

case in C3 plants. An international C4 rice consortium with the aim to bioengineer C4 photosynthesis in rice began in 2008 (see <https://c4rice.irri.org/>), and significant progress has already been made to identify genes that are involved in the NADP-ME-type C4 pathway, and to successfully introduce some of these into rice, as published by Ermakova et al. (2020, 2021). On the other hand, important modelling work is needed in order to verify different hypotheses related to the various ways to proceed in this endeavor, and to regulate the functionality and viability of such radical changes that control morphological and biochemical conversion in rice photosynthesis. In this direction, Ermakova et al. (2020) have used a combination of the C3 model of photosynthesis by Farquhar et al. (1980) and the enzyme-limited C4 model of von Caemmerer (2000), showing that even small amounts of C4 photosynthesis introduced around the existing veins in rice could enhance photosynthesis. This is consistent with the results obtained by Wang et al. (2017a, b), in which a 3D reaction diffusion model of connected M and BS cells in a C3 rice leaf was used to answer the question: Would the photosynthetic efficiency be improved by expressing C4 metabolism into a C3 leaf structure, without removing the C3 background metabolism? Data of Wang et al. (2017a, b) show that this is indeed possible, but in the engineered C3–C4 leaf, the partitioning of the energy between C3 and C4 photosynthesis, and that of Rubisco between the M and BS cells, are the main factors that would control the photosynthetic efficiency. Furthermore, Bellasio and Farquhar (2019) have used a leaf-level biochemical model for C3, C2, C2 + C4 and C4 photosynthesis (cf. Bellasio 2016) to simulate the introduction of C2 and C4 photosynthesis in C3 rice. Besides the ATP-limited and NADPH-limited sub-model of CO<sub>2</sub> assimilation, the above-mentioned model contains a hydromechanical and biochemical sub-model of stomatal conductance, and a mechanistic description of light reactions necessary to simulate the NADPH and ATP generation, including cyclic electron flow around PSI that can be engaged, variably, to regulate the NADPH/ATP ratios. The simulations with this model have shown that C4 photosynthesis becomes detrimental under low light, at low temperature, and at high [CO<sub>2</sub>], which agrees with the available ecophysiological observations. Additionally, Wang et al. (2021) have studied the limiting factors of the C4 photosynthesis under non-steady-state conditions, by combining gas exchange data on maize, sorghum, and sugarcane (obtained under fluctuating light regimes) with a dynamic C4 photosynthesis model including dynamic stomatal conductance, post-translational regulation of key photosynthetic enzymes (with their temperature responses), and leaf energy balance. By comparing their model outputs with the rates of CO<sub>2</sub> uptake and leaf stomatal conductance, Wang et al. (2021) showed that Rubisco activase, pyruvate phosphate dikinase regulatory protein, and stomatal conductance are the major

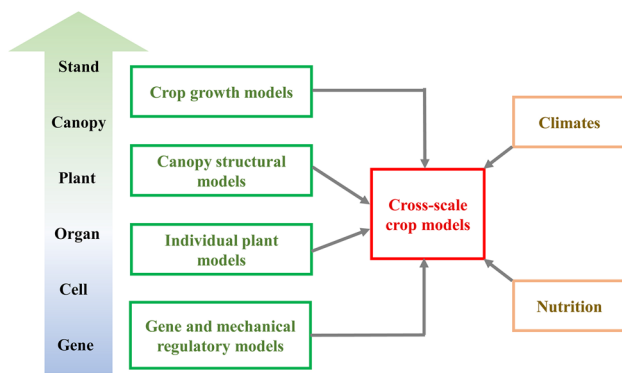
limitations for the efficiency of the NADP-ME-type C4 photosynthesis during dark-to-high light transitions, which indicates that these components are good possible bioengineering targets for increasing photosynthesis in some C4 crops.

## Models are imperative for improving crop yield

For the improvement of crop yields, canopy models are crucial, as they are key to not only basic long-term research on crop productivity, but also for applied research that provides short to medium term predictions at both field and subfield scales. Crop models can be of different types, depending on their design, such as empirical (e.g., correlative or statistical), and process-based models, which require physiological data from field experiments for parameterization (see e.g., Kasampalis et al. 2018). The process-based crop growth models describe the photosynthesis of the entire crop field, as well as the daily and seasonal integrals of CO<sub>2</sub> assimilation rate of the canopy ( $A_c$ ), which are correlated positively with daily and seasonal biomass production (X-G. Zhu et al. 2012, 2013; Song et al. 2017). Several types of canopy models have been developed to realistically simulate canopy photosynthesis under heterogeneous microenvironments, such as the *big leaf model* (Sellers et al. 1996), the *sunlit/shaded model* (De Purry and Farquhar 1997; Wu et al. 2018), and the *3D canopy photosynthetic model* (Song et al. 2013; Liu et al. 2021). Additionally, the architecture of the crops—such as plant height, plant density, spike length, spike height, position in the canopy, and leaf angle—is a major factor that influences canopy photosynthesis and crop yields (see e.g., Song et al. 2017; Chang et al. 2022). For example, Chang et al. (2022) found that, in general, shorter plant height, erect leaves, lower spike position, and appropriate plant densities can improve the daily  $A_{c_{net}}$ .

As mentioned earlier in the paper, increasing photosynthesis is an important target to increase crop productivity (Long et al. 2006; Evans 2013; Long 2014; Ort et al. 2015; Furbank et al. 2020; Zhu et al. 2010, 2022; Walter and Kromdijk 2022). For this reason, model-guided genetic modifications (von Caemmerer et al. 2012; South et al. 2019; Ermakova et al. 2020), and model-guided natural variations of the photosynthetic parameters (Qu et al. 2017; Ye et al. 2019; Yin et al. 2022) have already been employed to promote crop yield growth.

Simple scale crop models can provide explanations for specific biological phenomena and are capable of guiding the development of measurement techniques, as well as providing suggestions for the modification of plant traits in a direction that is beneficial for the humankind. However, these models cannot track key interactions and gaps resulting from the complex system characteristics, especially the



**Fig. 6** Basic framework for cross-scale modelling

nonlinear behavior that may appear through the feedback of the interaction of crop growth, interspecific competition, and dynamic micro-environments (Qu et al. 2011; Wu et al. 2019). Several studies have, however, already shown that the effect of manipulating photosynthesis can become weaker at the canopy scale, because of the complexities in the light interception process at the canopy level (Zhu et al. 2012; Song et al. 2013; Yin and Struik 2017; Wu 2023; Wu et al. 2016, 2018, 2019, 2023); in fact, light absorption, even by a single leaf, is a nonlinear function, see e.g., Baránková et al. (2016) and Nauš et al. (2018). In addition, nitrogen deficiency has been shown to reduce the yield-enhancing effects of increased CO<sub>2</sub> on photosynthesis as well as growth (Wu et al. 2019). Therefore, cross-scale crop growth models should prevail in crop modelling, as they can reveal new, the so-called emergent features that cannot be “seen” by a simple scale model, obtained by the interaction of models at different spatial and temporal scales (Fig. 6). Indeed, the crop mechanistic models should integrate seamlessly the multiscale physical and molecular processes in the crops, by including sub-models of different processes of crop growth and development in cells, tissues, organs, individual plants, and even the entire crop (see Xiao et al. 2017; Chang et al. 2019a; Hammer et al. 2019). Further, the crop models may also contain different types of data, depending on the goal of the study (see e.g., Xiao et al. 2017; Benes et al. 2020). For example, there can be (i) crop models which include remote sensing data (Kasampalis et al. 2018); (ii) spatialized crop models, from small fields to global level (Pasquel et al. 2022); (iii) metabolic engineering models (Cavanagh et al. 2022); and (iv) systems models including phenomics, genomics, and/or high-throughput photosynthetic measurements data (Chang et al. 2019b; Baslam et al. 2020; Yin et al. 2022).

Figure 6 shows the basic framework of a cross-scale model, from the genes to the stand; further, it incorporates information on the climate and the nutritional factors. Such models not only help us visualize the physiological state of

the crops but allow us to predict how the growth and the development of plants may respond, comprehensively, to different environmental signals (Lynch 2007); in addition, they can guide the experimental design and the technology development to increase crop yields and to ensure that the crops grow in suitable environments (see e.g., Srinivasan et al. 2017).

At present, cross-scale crop growth models are widely used to study the response mechanisms of crop productivity under different environmental and management conditions, and to explore potential ways to improve crop yields (Benes et al. 2020; Chang et al. 2022; Wu et al. 2016, 2018, 2019, 2023). For example, the CERES (Crop Environment Resource Synthesis) model ranges from gene-based modelling, nutrient and water stress, farm and precision management to regional assessment of climate change impacts. This cross-scale system model has been widely used in the analysis of agricultural experiments, in yield forecast, and in production risk assessment (Jones et al. 2003). Also, APSIM (Agricultural Production System Simulator) is a modular crop system model that is used to simulate the biophysical processes in agricultural systems. We note that APSIM allows independent modules describing the key components of agricultural systems to be “plugged” into the platform, so that the ‘master-model’ becomes suitable for relatively accurate prediction of the crop yield under different conditions, under different climate, soil, and management factors, while analyzing long-term water resource management issues (Brown et al. 2014; Holzworth et al. 2014).

Table 1 is a summary of what is known, as well as the differences between the four commonly used cross-scale crop growth models, namely WOFOST (World Food Studies), Aqua Crop, CERES (Crop Environment Resource Synthesis) and APSIM (Agricultural Production Systems Simulator). In addition, the cross-scale crop growth models have been widely used in optimal management studies under different stress conditions, such as water stress (Yang et al. 2017; Wang et al. 2017a, b; Zhuo et al. 2022), nutrient stress (Shibu et al. 2010; Saengwilai et al. 2014; Galindo-Castaneda et al. 2018), and weather stress (Rosenzweig et al. 2013; Gabaldón-Leal et al. 2016; Rincent et al. 2019). The key to establish a cross-scale crop model is to have a series of basic data, including soil properties and crop parameters. However, there are difficulties in obtaining and calibrating some of the model parameters. At present, most parameters of crop system models are default or empirical parameters, which often lead to deviations in the accuracy of the model simulation. In addition, as a complex system model, the cross-scale crop models require verification and evaluation of experimental data to describe the rationality of its single processes and the interaction relationship between the various processes. The current acquisition of crop characteristics is mostly based on their manual measurement, which is

**Table 1** Summaries and differences of four typical crop growth models: WOFOST (World Food Studies), Aqua Crop, CERES (Crop Environment Resource Synthesis), and APSIM (Agricultural Production Systems Simulator)

Model	Development agencies	Module composition	Features	Applications
WOFOST (World Food Studies)	Wageningen Agricultural University The Center for World Food Studies	Assimilation module; Respiration module; Transpiration module; Crop growth period; Soil moisture balance; N, P, K nutrient limitations	Universal applicability: it can be applied to different crops, just by adjusting the crop parameters; Note: too many crop parameters can be problematic	Prediction of crop yield variation (Ma et al. 2013; Boogaard et al. 2013) Climate change risk analysis (Gilardelli et al. 2018; Biswas et al. 2018) Quantitative land evaluation (Cheng et al. 2018; Zhu et al. 2018)
Aqua Crop	FAO	Crop phenology; Canopy cover; Crop transpiration; Soil transpiration; Canopy coverage	Use canopy coverage instead of leaf area index, with fewer input parameters Lack of crop physiology submodule	Optimizing irrigation regimes and evaluating management practices (Wellens et al. 2013; Nyakudya and Stroosnijder 2014) Impact of climate change on yields (Lorite et al. 2013; Soddu et al. 2013)
CERES (Crop Environment Resource Synthesis)	USDA-ARS Michigan State University	Soil moisture balance; Nitrogen balance; Phenological development process; Crop growth process	Consider the Genetic characteristics of the crops	Large area yield forecasting (Ghosh et al. 2015; Li et al. 2016) Crop variety breeding (Adnan et al. 2019)
APSIM (Agricultural Production Systems Simulator)	APSRU	Crop physiology module; Soil processes including pH, erosion processes Water balance module; Nutrient modules, such as N and P	The core of the model is soil, which mainly considers the impact of weather and management measures on soil Modular design, strong scalability; High sensitivity under extreme conditions	Regional water balance (Connolly et al. 2002; Amarasingha et al. 2015) Impact of climate change on yield (Pemberton et al. 2016; Bahri et al. 2019) Land use (Luo et al. 2014; Cichota et al. 2021) Crop breeding (Chapman et al. 2003)



time-consuming, and laborious. Further application of spectral technology, agricultural big data, agricultural internet of things, computer vision technology, and citizen science approach will, in the future, make it easier for the acquisition of crop characteristics.

For overcoming the challenges ahead of us, further research in modelling is essential, especially by using advances in promising and fast developing domains, such as artificial intelligence (see e.g., Xia et al. 2023) and remote sensing (RS) techniques (Kasampalis et al. 2018; Zhou et al. 2022). Since the climate change is affecting the agriculture through increased temperature and atmospheric CO<sub>2</sub> concentration, as well as by modification of the weather patterns, it is important to monitor the status of growth during the entire lifecycle of the crops, as it can provide valuable information on the ‘health’ and the yield potential of the crops. Remote sensing (RS) has already proven to be an effective method for monitoring crop growth and for the estimation of the yield, due to its ability to provide large-scale, non-destructive, low-cost, and highly efficient approach to monitor crops (see e.g., Abdulridha et al. 2019; Mahlein et al. 2019). However, solar-induced (chlorophyll) fluorescence (SIF) is a much more accurate way to measure the photosynthetic activity of plants than the traditional indices of RS, such as the Normalized Difference Vegetation Index (NDVI), the Enhanced Vegetation Index (EVI), the Photochemical Reflectance Index (PRI) and the Leaf Area Index (LAI), which are only slightly sensitive to the actual photosynthesis (Meroni et al. 2009; Zhang et al. 2016; Song et al. 2020). For example, Pandiyan et al. (2021) have successfully used the SIF signal to monitor the effect of drought on photosynthesis. Further, Guanter et al. (2014) showed that SIF is highly correlated with the gross primary production (GPP) and is much more sensitive to environmental changes than the other indices mentioned above (see also Frankenberg and Berry 2018). Thus, SIF has a distinct advantage in obtaining information on photosynthesis and in predicting crop yield, especially under the climate change (Peng et al. 2020). Further, Magney et al. (2019) have concluded, based on the interpretation of SIF signals, that the wavelengths used by satellites are stable enough to even track the downregulation of photosynthesis resulting from stress, while spectral shape changes respond more strongly to dynamic changes in canopy structure and chlorophyll concentration. An example in this direction has been the use of hyperspectral imagery and SIF retrievals from aerial and satellite remote sensing for the detection of variations in the rates of photosynthesis in many crops (Camino et al. 2019).

Finally, although the current satellite SIF data have relatively low spatial resolution, which limits their accuracy in estimating crop yield at finer scales (Zhang et al. 2019), a convolutional neural network (CNN) framework has been proposed by Kang et al. (2022) to downscale the SIF data

from a resolution of 0.05° to 0.0005°. This newer method has been quite effective, the results showing a high level of agreement with the referenced SIF (i.e., the spatial continuous SIF; see Kang et al. 2022). This research emphasizes the significance of using higher resolution SIF data (i.e., CNN-SIF) to obtain precise crop yield estimates, particularly for farms that are not contiguous. Further, by using other remote sensing indices together with SIF to predict crop yields, it is possible to obtain better results than by using only one alone (Liu et al. 2022). Therefore, we suggest that it is essential to conduct further research to evaluate the effectiveness of high-resolution SIF data in predicting yields of various crops. A new satellite called FLEX (Fluorescence Explorer) by European Space Agency is planned to be launched in 2025; it has been designed especially for the high-resolution detection of SIF (see <https://earth.esa.int/eogateway/missions/flex>) should be helpful in this.

**Acknowledgements** GG thanks Jeff Haas; Karl Schlieff; and Tom Uebele, of the Life Sciences Office of Information Technology at the University of Illinois at Urbana-Champaign for computer-related help. YG was supported by the Natural Science Foundation of China (No: 51961125102, No: 31771680), Jiangsu Agricultural Science and Technology Innovation Fund (SCX(22)3669). DL was supported by European Regional Development Fund project ‘Plants as a tool for sustainable global development’ (CZ.02.1.01/0.0/0.0/16\_019/0000827) and by European Innovation Council, HORIZON-EIC-2021-PATHFINDER OPEN project DREAM (Grant Agreement No. 101046451).

**Author contributions** All the authors (AS, YG, DL and GG) contributed to the writing and the editing of this manuscript; figures were prepared by AS.

**Data availability** Data will be made available, if required.

## Declarations

**Competing interests** The authors declare no competing interests.

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