Integrating Leaf and Canopy Photosynthesis Modelling for Enhanced Crop Improvement

Pengpeng Zhang and Youhong Song

***Abstract*—Predicting crop yield by integrating molecular basis for crop improvement attracts increasing interest but remains a great challenge due to complex biological and physiological processes across various scales. Crop physiological models have been developed and successfully used in predicting crop growth, development, and grain yield formation in response to various environments for more than half century. The crop model realized a chain of non-linear processes from canopy development, canopy photosynthesis, biomass growth and allocation, grain yield formation, and nitrogen, water, and energy balance based on detailed physiological and agronomic experiments. On the other hand, leaf biochemical photosynthesis was also modelled with relatively simple equations four decades ago, which receives wide attention due to underlying explicit biochemical mechanisms. Apart from that, the model is based on photosynthetic events occurring on leaf cellular chloroplast, which more closely represents the fundamental molecular regulation. Molecular regulatory network of photosynthesis is made clear, but such achievement in improving grain yield has not been translated well in that the molecular basis is not directly reflected in whole plant performance and lacking predicting ability from cellular level to whole plant level. Consequently, connecting both types of models will greatly accelerate the efforts of realizing the prediction of molecular outcomes in grain yield formation. Here we reviewed development of leaf and canopy photosynthesis models, and discussed the connection of both types of models to support crop improvement.**

***Index Terms*—Crop improvement, canopy photosynthesis, leaf biochemical photosynthesis, crop models, model connection, molecular basis, whole plant physiology**

I. INTRODUCTION

A. Mission Switch in Crop Improvement

CROP yield depends on resource capture by plant, resource use efficiency, and harvest index. While extensive efforts to optimize resource capture and harvest index have brought crop productivity to a plateau with narrow margins for further enhancement [1], our grasp of the physiological and molecular mechanisms regulating resource dynamics—including capture, flow, and utilization—has advanced profoundly. Therefore, shifting the focus toward elevating resource use efficiency represents a promising new frontier for driving advancements in agricultural productivity [2].

B. Photosynthesis Offers Potentials for Crop Improvement

Through the process of photosynthesis, leaves intercept solar radiation and convert it into chemical energy by transforming carbon dioxide into stored carbohydrates. As a fundamental cellular biochemical pathway, leaf photosynthesis serves as the primary stage where critical resources (i.e., light, water, and nitrogen) are integrated, making it a pivotal target for optimizing resource use efficiency. Carbon assimilation within the leaf acts as the foundational energy source that drives crop growth, development, and yield formation. Research has demonstrated that leaf photosynthesis can be significantly boosted either by elevating CO_2 concentration or by optimizing the performance of key photosynthetic enzymes [3, 4]. Consequently, optimizing the biochemical activities of the photosynthetic process presents a significant opportunity for elevating crop productivity [5–8].

Enhancing photosynthetic capacity is considered a pivotal strategy for boosting agricultural productivity to meet the demands of expanding populations [5]. The clarification of photosynthetic biochemical pathways [9] boosts the currently processes of photosynthesis improvement. Since CO_2 is the raw material for carbon fixation, minimizing diffusion barriers is a top priority, specifically through the regulation of stomatal [10] and mesophyll conductance [11]. Under field conditions, the photosynthetic capacity of leaves is typically capped by electron transport limitations or the ability to harness the produced chemical energy [5]. In the context of light reactions, potential enhancements include extending the usable spectrum into the near infrared radiation (NIR) [12], optimizing canopy light distribution by reducing antenna sizes in top leaves [13, 14], and facilitating a faster relaxation of photoprotective heat dissipation at photosystem II (PSII) [15–17]. When light is non-limiting, carbon assimilation is often co-limited by the efficacy of the carboxylation step and the replenishment of its substrate [5].

Downstream processes in the dark reactions offer multiple targets for optimization, such as engineering C4 traits into C3 species [8], incorporating inorganic carbon-concentrating mechanisms from algae or cyanobacteria [18, 19], redesigning rubisco for current CO_2 level [20], and synthetizing photorespiratory bypasses [21, 22]. Furthermore, enhancing ribulose bisphosphate (RuBP) regeneration [23] and improv-

Manuscript received: 11 February 2026; revised: 9 March 2026; accepted: 18 March 2026. *(Corresponding author: Youhong Song.)*

Citation: P. Zhang and Y. Song, Integrating leaf and canopy photosynthesis modelling for enhanced crop improvement, *Int. J. Intell. Control Syst.*, 2026, 31(1), 42–52.

Pengpeng Zhang is with Institute for Crop Sciences, Chinese Academy of Agricultural Sciences, Beijing 100081, China (e-mail: pp_zhang0413@163.com).

Youhong Song is with School of Agricultural Sciences, Jiangxi Agricultural University, Nanchang 330045, China, and also with Centre for Crop Science, Queensland Alliance for Agriculture and Food Innovation, The University of Queensland, Brisbane QLD 4350, Australia (e-mail: y.song@jxau.edu.cn; y.song@uq.edu.au).

Digital Object Identifier 10.62678/IJICS202603.10306

ing light penetration to the lower canopy [24, 25] can also boost performance. While certain strategies currently appear more feasible, there is insufficient evidence to prioritize one specific method, as many of these targets have yet to test through field-based validation.

C. Limited Predictive Ability from Molecular and Biochemical Basis to Crop Yield

Crop yield does not always mirror the molecular drivers of leaf photosynthesis, as numerous non-linear processes govern the transition between cellular biochemical activities and yield. Consequently, efficient modeling tools are indispensable for evaluating and predicting the impact of molecular-scale modifications on whole-plant performance [26–28]. Additionally, the scientific consensus among physiologists is that crop yield represents a highly complex phenotype, where leaf-level carbon fixation is only one of many contributing physiological factors [8, 27]. This suggests that future breeding efforts should focus on identifying diverse trait variations and integrating them in a synergistic manner to achieve substantial yield gains.

D. Existing Basis for Modelling Prediction

Since 1965, canopy photosynthesis modelling has evolved into a comprehensive system capable of integrating environmental and management-related factors [29]. As the fundamental engine for plant growth and development within crop models, the underlying algorithms for canopy photosynthesis have shifted from empirical light-response curves [29] or biomass-light efficiency correlations [30] toward more mechanistic biochemical frameworks at the leaf level [28, 31]. These biochemical models offer a high-fidelity simulation of plant-environment dynamics, bridging the gap between molecular and multi-organismic scales [5].

With current scientific insights, it is now feasible to construct virtual crop canopies [26, 32]. Such models function as testing grounds for hypotheses aimed at maximizing carbon sequestration and applying optimization strategies for improved efficiency. To date, numerous mechanistic modules have been refined, encompassing gene regulation [32], photosynthetic biochemistry [33], mesophyll-cell diffusion dynamics [34], stomatal behavior [10], respiration [22, 35], and complex 3D microclimates within the canopy [36]. Despite their utility in identifying specific pathways for improvement, these isolated frameworks often fail to account for the interactions occurring within the entire plant system or the surrounding environment. The integration of these diverse modules into a multi-scale modeling framework can facilitate more accurate, system-wide predictions of photosynthetic performance across different biological levels.

E. Objectives of This Literature Review

To this end, this study first reviews the evolution of both canopy-level and biochemical-scale photosynthesis simulations. Subsequently, it evaluates the adaptability of these models in light of emerging scientific missions and constraints. Finally, we elucidate potential methods for synthesizing these two modeling paradigms to provide a robust theoretical foundation for crop improvement initiatives.

II. MODELLING CROP CANOPY PHOTOSYNTHESIS

Defined as the aggregate photosynthetic activity of all leaves in a stand, canopy photosynthesis captures the dynamic interactions occurring among plants and their external surroundings at the population scale, which functions as a foundational metric for estimating agricultural productivity [28] and plays a significant role in modulating global climate patterns by regulating atmospheric CO_2 levels [37]. The light dependence of a canopy deviates significantly from that of a single leaf; thus, canopy photosynthesis cannot be accurately estimated by merely aggregating the photosynthetic rates of all leaves [38]. Within the canopy, the carbon assimilation capacity of individual leaves is dictated by their placement, physical form, and physiological status [39]. Environmental variables inside the canopy, including the intensity and spectral composition of light, temperature, moisture levels, and CO_2 gradients, display pronounced spatiotemporal variability [36, 40, 41]. In addition to structural differences, leaves exhibit marked physiological divergence across the canopy profile [7]. Specifically, upper canopy leaves are characterized by increased rubisco content and leaf thickness, as well as higher chlorophyll a to chlorophyll b ratios, whereas lower leaves show different protein and pigment compositions [13, 42]. It is essential to recognize that leaves undergo developmental acclimation to their local light environment over time. Such adaptive plasticity in photosynthetic metabolism is particularly evident in shade-tolerant plants responding to intermittent light patches [43]. Despite the abundance of existing canopy models, only a limited number of them incorporate the intricate physiological variations and specific performance of each leaf. Accounting for these factors is necessary to ensure that modeled canopy gas exchange remains consistent with measured data.

A. Maximum Productivity Model

As the most rudimentary approach to simulating canopy net primary productivity (NPP), the maximum productivity model calculates output by adjusting a crop-specific potential maximum. This adjustment accounts for limiting environmental stressors such as insufficient light, sub-optimal temperatures, and the scarcity of water or nutrients [44].

The CENTURY model, frequently employed for simulating soil organic matter dynamics, adopts this simplified logic [44]. Given it focuses on underground carbon processes, the model avoids complex photosynthetic architectures [45]. However, this trade-off prevents the simulation of crop responses to varying levels of incident light. When applied at the site level, the model's reliability has been verified across diverse ecosystems, ranging from grasslands [46] to forests [47]. Findings suggest a satisfactory performance, with deviations typically remaining within ±25% of empirical measurements [48]. Nevertheless, because the datasets for calibration and validation frequently overlap [46], these results may not constitute a truly stringent assessment of the model's predictive accuracy. Similar to the maximum productivity approach, several other frameworks utilize coarse-grained techniques for canopy-scale simulations. Notable examples include terrestrial ecosystem model (TEM) [49], PnET [50], and integrated biosphere simulator (IBIS) [51], all of which are extensively applied to study productivity within terrestrial ecosystems.

B. Radiation Use Efficiency (RUE) Model

Rooted in early efforts to correlate crop weight with solar radiation [29], the RUE model emerged from the documented linear relationship between cumulative intercepted light and dry matter production [52]. This concept has since been consolidated through extensive experimental and theoretical verifications [53]. Consequently, RUE is the biomass generated per unit of total radiation or photosynthetically active radiation (PAR), and has become a pivotal metric in productivity analysis and a core of crop growth simulation. In practice, canopy productivity is estimated by taking the product of the light intercepted (derived from light distribution models [54]) and a predefined RUE [55]. The RUE can be obtained by fitting a linear relationship between cumulative biomass accumulation and cumulative radiation interception.

Thereafter RUE has quickly received much interest and many studies carried out in determining RUE values in various crop species and environments. Variations in RUE are primarily determined by crop type, with C4 plants exhibiting the highest capacity, followed by non-legumes and legumes [55]. Furthermore, RUE is not a static constant; it is sensitive to nitrogen status [56] and light quality. Evidence suggests that a shift toward diffuse radiation can boost RUE by up to 50% in various species [57, 58]. The widespread adoption of RUE in diverse crop models is primarily attributed to its straightforward formulation and the relative ease of obtaining its governing parameters. A theoretical challenge within the RUE approach involves the mechanism by which non-linear leaf-level light responses are effectively scaled into a linear canopy-level representation. Evidence indicates that this linearity is an emergent property applicable only at two weeks or longer intervals, whereas the coupling between intercepted radiation and productivity remains non-linear on a short-term scale [59, 60]. Furthermore, synergistic interactions among multiple resource constraints contribute to the observed long-term linearity of light-limited canopy photosynthesis [61]. For instance, under nitrogen-deficient conditions, RUE is positively with leaf nitrogen concentration [56] and is sensitive to the vertical distribution of nitrogen within the canopy profile [62]. RUE values for maize, soybean, and grass have been reported to rise by 33%–50% when the light environment shifts toward lower total incident radiation but higher diffuse radiation [57, 58]. Echoing the sensitivities of leaf photosynthesis, RUE fluctuates in response to temperature, CO_2 concentration, and water availability [28]. Therefore, RUE-based models typically employ corrective functions to account for these environmental constraints and improve predictive robustness [63].

The aforementioned methods represent simplified frameworks for estimating canopy photosynthesis. Both the maximum productivity and RUE models were conceptualized through a "top-down" lens, grounded in empirical observations at the macroscopic scale, with their linkages to microscopic processes being explored only retrospectively. Consequently, these models necessitate a vast array of empirical coefficients to encapsulate the influences of fluctuating environments and intrinsic plant physiology. This heavy reliance on empirical fitting serves as a major constraint on their predictive precision. Although effective for assessing photosynthetic potential within specific conditions, these approaches lack the robustness required for extrapolation to novel environments. Their primary deficiency lies in an inability to resolve the intricate interactions between canopy photosynthesis and external drivers, such as temperature, humidity, or CO_2 concentrations [26, 64]. As a result, such modeling paradigms may prove inadequate when the objective is to evaluate the consequences of physiological modifications or rapidly changing climatic scenarios.

C. Multi-Layer Approach

The inception and advancement of empirical frameworks for canopy photosynthesis were primarily driven by the formulation of mathematical leaf light-response curves. Concurrently, the integration of light attenuation models within the canopy significantly catalyzed the growth of this field [54]. The multi-layer framework operates by partitioning the whole canopy into numerous horizontal layers. Early versions of these models utilized exponential functions, such as the Beer-Lambert law, to simulate vertical light gradients. The extinction coefficient (k) is determined for different canopies primarily based on leaf inclination angles [54]. A key simplifying assumption of this approach is that all leaves within a given horizontal layer experience uniform light availability. The light-response behavior of individual leaves was typically represented by a rectangular hyperbola function. The canopy photosynthesis is the sum of individual leaf photosynthesis rates. This framework proved effective in providing a formal mathematical description of the essential drivers of canopy photosynthesis.

A subsequent development was a simplified multi-layer canopy model [65] that focused on vertical variations in wind speed and irradiance. However, it treated other environmental factors as uniform across whole canopy, including temperature, humidity, and CO_2 concentration. Almost at the same time, an advanced multi-layer framework was introduced [66] with expanded capabilities. It facilitates the calculation of real-time CO_2, heat, and radiation, allowing canopy photosynthesis to be estimated through empirical models of light absorption. Despite their inherent complexity, full multi-layer models serve as powerful tools for both modeling energy and mass exchange between canopy and the atmosphere and elucidating the underlying physiological and physical mechanisms.

Early modeling efforts assumed leaf homogeneity across the canopy due to limited computing resources. To incorporate vertical physiological gradients, researchers began by calculating leaf nitrogen profiles within the canopy and linking them to key light-response parameters [67]. While initial leaf photosynthesis model relied solely on light as a driving variable, the emergence of biochemical modeling [33] allowed for the simultaneous consideration of CO_2 and temperature. The subsequent addition of stomatal conductance functions [68] created a synergistic approach for predicting leaf-level gas exchange in varying environmental conditions [69, 70].

D. Big-Leaf Approach

The big-leaf model conceptualizes the entire canopy as a unified, single-layer leaf. This approach is predicated on the hypothesis that the spatial allocation of photosynthetic capacity throughout the canopy mirrors the gradient of light intensity [71]. Such a premise facilitates the direct scaling up of leaf-level light-response functions to the canopy scale. Additionally, it operates under the simplification that environmental variables, such as temperature and humidity, remain uniform across whole canopy. Consequently, the physiological reactions of the canopy to external drivers can be simulated via mechanistic biochemical models of leaf photosynthesis. This logic was pioneered by Farquhar [72], who stated that if leaf photosynthetic capacity is distributed proportionally to absorbed radiation and leaf-level response curves are consistent, the mathematical expressions for canopy carbon fixation retain the same structure as those for single leaves. This theoretical framework was promptly adopted and expanded within the domain of canopy photosynthesis research [71, 73].

Following this theory, various researchers have explored whether a vertical, exponential decline in leaf photosynthetic capacity occurs in tandem with radiation attenuation, following the principles of Beer's law. Given the robust linear correlation between leaf photosynthesis and leaf nitrogen levels [74], empirical validation has largely centered on the spatial partitioning of nitrogen within the canopy profile. Findings from optimization analyses demonstrate that nitrogen distribution in proportion to the light extinction represents a theoretical optimum for maximizing canopy carbon gain [71, 75]. It has been widely documented that leaf nitrogen and its corresponding photosynthetic capacity exhibit a marked downward trend along the vertical canopy axis [67, 76]. Model-based comparisons revealed that when total canopy nitrogen is conserved, the optimized nitrogen distribution closely mirrors observed patterns, suggesting that plants naturally tend toward this high-efficiency allocation strategy [67, 74].

Although the premise of a proportional reduction in photosynthetic capacity alongside light attenuation simplifies the integration of leaf-level models into canopy level, historical application has shown that it has not simplified integration. For example, the HYBRID model fails to account for diurnal fluctuations in canopy photosynthesis, relying instead on daily mean values for both irradiance and carbon fixation [77]. Consequently, this method disregards the critical interplay between the non-linear dynamics of leaf-level response models and the temporal variability of light absorption within the canopy structure. Nevertheless, even without internal parameter recalibration, the HYBRID model's efficacy was evaluated against global primary productivity and carbon stocks [78]. While the model exhibited satisfactory overall performance, certain inconsistencies with observations underscored specific domains necessitating refinement.

The big-leaf framework was later refined to include diurnal variations in solar radiation [79], leading to its successful implementation in models such as PROMOD [80] and CenW [81]. These models have undergone rigorous field-scale validation. For instance, PROMOD's predictive accuracy regarding annual increments was confirmed across 28 sites [80], while CenW was validated using experimental data on leaf nitrogen, soil moisture, and biomass partitioning from irrigation and fertilization trials [81]. A primary merit of the big-leaf approach is its compatibility with remote sensing data for light interception, which bypasses the complexity of simulating radiation transfer. This feature is leveraged by the simple biosphere model, version 2 (SiB2), which serves as the terrestrial surface module for the global climate model (GCM) [82]. Consequently, the model must function at high temporal resolutions (minutes) on a global scale. At such scales, incorporating the non-linear relationship between intercepted radiation and canopy photosynthesis becomes essential, making the big-leaf approach an appropriate modeling selection.

As previously noted, this approach is predicated on the assumption of a parallel exponential decline in both light intensity and leaf photosynthetic capacity within the canopy. Although this premise is technically an oversimplification, its practical application typically avoids introducing severe errors. A critical flaw is that leaf within any given layer comprises both sun and shaded leaves, each subjected to distinct light intensities [83]. Given the high temporal variability of sunlit leaves, the capacity for photosynthesis cannot be considered a simple linear function of the instantaneous light intensity. It is therefore imperative to partition the canopy into sunlit and shaded fractions, calculating their photosynthetic contributions independently. Empirical evidence from eddy covariance studies further indicates that canopies react differently to diffuse versus direct solar fluxes, necessitating a different modeling approach [84]. Both the heterogeneity of leaf exposure and the nature of incident light are explicitly accounted for in sun-shade modeling framework.

E. Sun-Shade Leaf Approach

The sun-shade leaf framework provides a comprehensive accounting of the distinct behaviors of direct and diffuse radiation, as well as the pervasive nature of diffuse flux within the canopy. Specifically, this modeling paradigm partitions the canopy into several layers, each of which is bifurcated into two distinct physiological populations: sunlit and shaded leaves. Within this approach, sunlit leaves are modeled as intercepting a combination of direct and diffuse radiation, whereas shaded leaves are restricted to diffuse-only interception. A foundational assumption of this approach is the spatial homogeneity of both radiation interception and photosynthetic activity within each leaf fraction [83]. By synthesizing the characterization of shaded leaves with the theory of optimal canopy nitrogen partitioning, a highly precise canopy photosynthesis model is realized [83, 85]. Building upon these premises, the sun-shade model [83] integrates a mechanistic biochemical model of leaf photosynthesis [33] to compute canopy-level CO_2 assimilation rates [33].

While the sun-shade model exhibits greater architectural complexity than the big-leaf approach, it maintains a mechanistic framework that does not necessitate additional parametric input. Its primary advantage is the strategic weighting of sunlit versus shaded leaf contributions, achieved by dividing the canopy into these two distinct physiological classes. Consequently, this model offers superior predictive accuracy relative to the previously discussed empirical and simplified frameworks. A notable constraint, however, is its incompatibility with radiation interception data derived from remote sensing, thereby demanding more comprehensive information for robust parameterization.

The initial implementation of the sun-shade leaf approach was featured in the generic decomposition and yield (G'DAY) model [86], utilizing photosynthetic parameters derived directly from in field measurements. Despite its foundational role, the initial scalability of this model remained limited, as it lacked extensive validation and application across broader geographical contexts. The adoption of the sun-shade leaf approach within G'DAY was primarily motivated by the facility with which leaf-level responses to nitrogen, water availability, and temperature could be integrated into the canopy framework. This represented a significant advancement over earlier iterations of the G'DAY model, which relied on the RUE paradigm [87]. A prominent example of upscaling the sun-shade leaf approach for regional net primary productivity simulations is the CSIRO biospheric model (CBM) [85]. Functioning at a 30 min temporal resolution, CBM provides high-frequency simulations of gas and energy exchanges within the soil-plant-atmosphere continuum. Site-specific validations using wheat eddy covariance data have demonstrated its predictive accuracy [85], leveraging established physiological parameters to refine the light-response curvature [88].

F. 3D Modeling Approach

Integrated as the driving force within crop simulation systems, canopy photosynthesis models quantify carbon fixation throughout the growing season [29]. These range from simple linear maximum productivity models and RUE models [52, 53] (e.g., light interception and utilization simulator (LINTUL) [59], agricultural production systems simulator (APSIM) [89], and decision support system for agrotechnology transfer (DSSAT) [90]) to more complex leaf-aggregation approaches like the multi-layer models, big-leaf models, and sun-shade leaf models [29, 91, 92] (e.g., simple and universal crop growth simulator (SUCROS) [93] and genotype-by-environment interaction on crop growth simulator (GECROS) [94]). While certain models like APSIM allow for algorithmic flexibility [95], most share a common limitation: an overly simplify canopy geometry. This lack of architectural detail precludes an accurate representation of internal environmental heterogeneity, rendering such models inadequate for evaluating structural modifications or identifying breeding targets for enhanced light interception.

Recent advancements in functional-structural plant models (FSPMs) have enabled the characterization of intricate spatiotemporal dynamics regarding plant growth within a 3D context. These provide a robust foundation for the high-fidelity simulation of light distribution within complex canopy architectures. Diverging from traditional approaches that rely on simplified parameters such as extinction coefficient or leaf area index (LAI), this 3D framework reconstructs the canopy by integrating granular architectural traits, including tiller and leaf counts, spatial positioning, and leaf orientation, with specific agronomic variables like planting density and row direction [96]. Subsequently, a ray-tracing algorithm is deployed, incorporating data on incident irradiance intensity, spectral composition, and angular directionality to compute the precise light intensity received by individual leaves within the canopy. By synthesizing these radiation inputs with leaf photosynthesis and stomatal conductance parameters, a comprehensive 3D canopy photosynthesis model is established. This framework serves as a versatile biophysical platform for the precise estimation of canopy photosynthesis. To empirically test the model's accuracy, a specialized canopy gas exchange measurement system was designed to provide direct observations of photosynthesis rates [97]. Comparative analyses demonstrated strong congruence between the simulated outputs and the observed data, confirming the model's predictive reliability.

A comparative study on canopy photosynthesis models with different dimensions demonstrated that crop yield predictions decreased by 12.0%–48.5% with increasing the resolution of light simulation [98]. However, the efficacy of the 3D canopy photosynthesis model depends on precise parameterization. Key requirements for this process include: (1) leaf-level biochemical and physiological parameters, such as maximum rate of rubisco carboxylation capacity and RuBP regeneration; (2) detailed architectural traits, such as tiller and leaf counts, leaf phyllotaxy, and leaf angle and orientation; and (3) agronomic configurations, including row spacing, plant density, etc. [96, 99]. These datasets can be acquired via traditional manual measurements or through advanced high-throughput phenotyping platforms. While manual characterization remains a labor-intensive and time-consuming bottleneck, it currently provides a baseline for model calibration. The rapid evolution of plant phenotyping technology is expected to mitigate the challenges of model parameterization. The 3D canopy photosynthesis model can provide more detailed structural and functional attributes of plants compared to other models; however, it entails greater effort in parameterization and is computationally expensive to execute [64]. Consequently, the selection between modeling approaches should be guided by the research objective: while RUE-based models are suitable for regional yield estimations due to their simplicity, 3D models are essential for identifying fine-scale breeding targets. As the technical barriers diminish in advanced genomics, phenomics, and computational, the 3D modeling approach will become an increasingly indispensable tool for crop improvement and understanding complex plant-environment interactions [100, 101].

The conceptual derivation of these canopy photosynthesis models follows two distinct paradigms. The big-leaf, multi-layer, sun-shade, and 3D modeling frameworks are rooted in a "bottom-up" approach, integrating fine-scale physiological non-linearities and their interactions with environmental drivers. Conversely, the maximum productivity and RUE methodologies adopt a "top-down" logic, derived initially from empirical measurements at the canopy scale.

Current canopy photosynthesis models demonstrate a high degree of biophysical realism, accurately capturing land-atmosphere exchange rates for carbon, water, and energy. Although these models range from mechanistic to simplified, they maintain remarkable predictive precision. The process of scaling up from leaf to canopy is fundamental to elucidating the mechanisms governing fluctuations in gas and energy exchange. Furthermore, these models are indispensable for projecting the long-term responses of terrestrial ecosystem functions to climate change. However, robust predictions depend on high-resolution data regarding plant architectural and functional traits. As the plasticity of these traits in response to changing environments remains partially obscured, current projections are often characterized by substantial uncertainties. Nevertheless, the synergy between expanding flux networks and improved data-model assimilation techniques is paving the way for more robust and sophisticated global carbon cycle prediction.

III. MODELLING BIOCHEMICAL PROCESSES OF LEAF PHOTOSYNTHESIS

Theoretical insights into leaf photosynthesis have culminated in the development of the Farquhar-von Caemmerer-Berry (FvCB) model [33], a cornerstone of C3 plant physiology. By mathematically representing the biochemical pathways within the chloroplast, the model estimates net CO_2 uptake A by identifying the primary limiting factor at any given moment. Specifically, it calculates A as the lower value between the rubisco-limited assimilation rate A_c and the electron transport-limited rate A_j.

$$A = \min\{A_c, A_j\} \tag{1}$$

A_c is calculated as a function of the maximum carboxylation capacity of rubisco V_{cmax} by Eq. (2).

$$A_c = \frac{(C_c - \Gamma_*)V_{\text{cmax}}}{C_c + K_c(1 + O_c/K_o)} - R_d \tag{2}$$

where C_c is the CO_2 partial pressure at the carboxylating sites of rubisco. K_c and K_o are Michaelis-Menten constants of rubisco for CO_2 and O_2, respectively. Γ_* is the CO_2 compensation point in the absence of day respiration R_d.

In the calculation of A_j, the FvCB model assumes 100% non-cyclic e-transport, thus excluding cyclic e-transport around photosystem I (PSI).

$$A_j = \frac{(C_c - \Gamma_*)J}{4C_c + 8\Gamma_*} - R_d \tag{3}$$

If adenosine triphosphate (ATP) supply is limited under 100% linear e-transport conditions, factors 4 and 8 in Eq. (3) are replaced by 4.5 and 10.5, respectively [102].

The C4 photosynthetic biochemical model [103] was developed based on the earlier researches [104, 105]. This model fundamentally adapts the core equations of the FvCB model to characterize the metabolic coordination between mesophyll and bundle sheath cells. The pivotal equations characterizing this process are presented as

$$A_c = \frac{(C_s - \gamma_* O_s)V_{\text{cmax}}}{C_c + K_c(1 + O_s/K_o)} - R_d \tag{4}$$

where γ_* is half of the reciprocal of rubisco specificity, C_s and O_s are the CO_2 and O_2 partial pressures in the bundle sheath, respectively.

$$A_j = \frac{(C_s - \gamma_* O_s)(1 - x)J_t}{3(C_s + 7/3\gamma_* O_s)} - R_d \tag{5}$$

where J_t is the whole-chain linear e-transport in the mesophyll and bundle sheath chloroplasts, and $(1 - x)$ is the partitioning fraction in the bundle sheath chloroplasts.

Since its original publication, the FvCB model has undergone significant evolutionary refinements. A notable limitation of the standard FvCB framework is its inability to account for the photosynthetic insensitivity to fluctuating CO_2 and O_2 concentrations observed under specific environmental conditions. This lack of response is attributed to the rate-limiting step of triose phosphate utilization (TPU) in the synthesis of starch or sucrose, which imposes a third metabolic bottleneck known as TPU limitation [106]. Intensive research into the CO_2 diffusion pathway has further revealed that carbon assimilation is constrained not only by biochemistry but also by stomata and mesophyll conductance [10, 11]. Advanced models, such as eLeaf, have integrated 3D CO_2 reaction-diffusion modules to quantitatively assess how internal leaf anatomy modulates photosynthetic capacity [107]. These studies highlight the critical role of leaf structural plasticity as a target for enhancing crop photosynthesis. Furthermore, to facilitate simulations across diverse thermal regimes, a multitude of temperature-response functions have been developed [108–110]. Through iterative refinements by the scientific community, the FvCB model has emerged as a highly successful tool, demonstrating exceptional reliability in fitting response curves and predicting leaf photosynthetic performance across most scenarios.

Beyond its foundational role in analyzing gas-exchange data [111, 112], the FvCB model has significantly advanced our understanding of electron transport regulation [113] and photosynthetic bottlenecks [114, 115]. By coupling this biochemical framework with stomatal control models [116, 117], researchers have successfully characterized the intricate balance between carbon gain and water loss [118]. Moreover, the model serves as a vital bridge for scaling physiological traits from the chloroplast to the canopy level [119]. This capability is particularly relevant for modern crop improvement, as it enables the quantitative evaluation of how metabolic engineering targets translate into tangible gains in biomass and yield [28, 120].

IV. NEW MISSIONS FOR CANOPY AND LEAF PHOTOSYNTHESIS MODELS

In modern crop models, RUE-based method can result in a 17% overestimation of carbon assimilation [121]. Most importantly, the "black-box" nature of these models precludes their use in identifying molecular targets for crop improvement [26]. To effectively support modern breeding, canopy photosynthesis module in crop models must evolve beyond empirical relationships to incorporate a mechanistic biochemical basis, effectively connecting molecular to whole-canopy productivity.

The engineering of the photosynthesis processes by biotechnologists must be supported by robust biochemical models. While advancements in biotechnology have transitioned traditional breeding toward molecular design breeding, significantly enhancing precision and accelerating cycles, breeders still struggle to identify multi-level physiological traits that effectively guide canopy photosynthesis improvements. Comprehensive canopy photosynthesis models empower researchers to identify diverse potential targets by scenario simulation across multiple scales. A prime example is the acceleration of recovery from photoprotection (non-photochemical quenching), which has been shown to substantially bolster both carbon assimilation and final yield [17]. Furthermore, optimizing leaf chlorophyll content via the reduction of light-harvesting antenna size not only maintains canopy photosynthesis by improving light penetration but also significantly enhances nitrogen use efficiency [13]. *In silico* prediction of crop performance is thus an essential prerequisite before physiologists initiate resource-intensive breeding programs [26, 122]. As a versatile tool for environmental impact assessment, multi-scale canopy modeling allows researchers to quantify the outcomes of specific metabolic or structural modifications [26, 123]. Given the prohibitive costs and logistical limitations of the free-air CO_2 enrichment (FACE) systems, the CoffeePlant3D model provides detailed insights into how coffee trees adapt both structurally and physiologically to carbon-rich atmospheres [124]. These 3D frameworks are particularly adept at characterizing the synergy between irradiance and gas exchange, offering a robust platform for climate-resilient crop design [125].

While existing models demonstrate exceptional performance at either the biochemical or canopy scale, empirical efforts to establish connectivity across these organizational levels remain limited (Fig. 1). To address this, a cross-scale modeling paradigm was pioneered [94], which successfully elevated FvCB model to the canopy scale by integrating the sun-shade leaf approach. Subsequent applications of this framework have enabled the quantification of potential yield gains from transitioning rice toward a C4 photosynthetic pathway [126], as well as the exploration of how utilizing natural genetic variation can enhance canopy productivity [127]. Furthermore, researchers have evaluated the biochemical bottlenecks limiting light-to-chemical energy conversion efficiency [128], and the impacts of improving photosynthetic properties on crop yield in Europe [120]. Utilizing this method, the revised APSIM model has successfully quantified the impacts of enhancing photosynthesis on crop yield across diverse environments in Australia [28, 129]. Similarly, applications of the revised GreenLab model identified maximal linear electron transport rate and light distribution are the primary limitations in high-density maize production systems [130].

Within this integrative process, coupling biochemical models with the spatiotemporal dynamics of crop development is imperative; without this linkage, simulations are restricted to transient daily predictions rather than seasonal trajectories [119]. Throughout the phenological cycle, foliage undergoes a transition from expansion to senescence, characterized by intricate feedbacks between photosynthetic capacity and internal physiological status [126]. Achieving a molecular-to-canopy modeling pipeline is now a critical priority for accelerating crop improvement in an era of global food insecurity.

V. CONCLUSION

Connecting leaf and canopy photosynthesis models has the capacity to link genetic manipulation of photosynthesis to crop yield. The prerequisite is to ensure that the models at each scale are reliable and effectively linked together. Scaling up the biochemical photosynthesis models to canopy level allows clearer links to the biochemical processes of photosynthesis, based on which consequences of photosynthetic manipulations can be reliably estimated. This can be further improved by the advancing understanding of photosynthetic

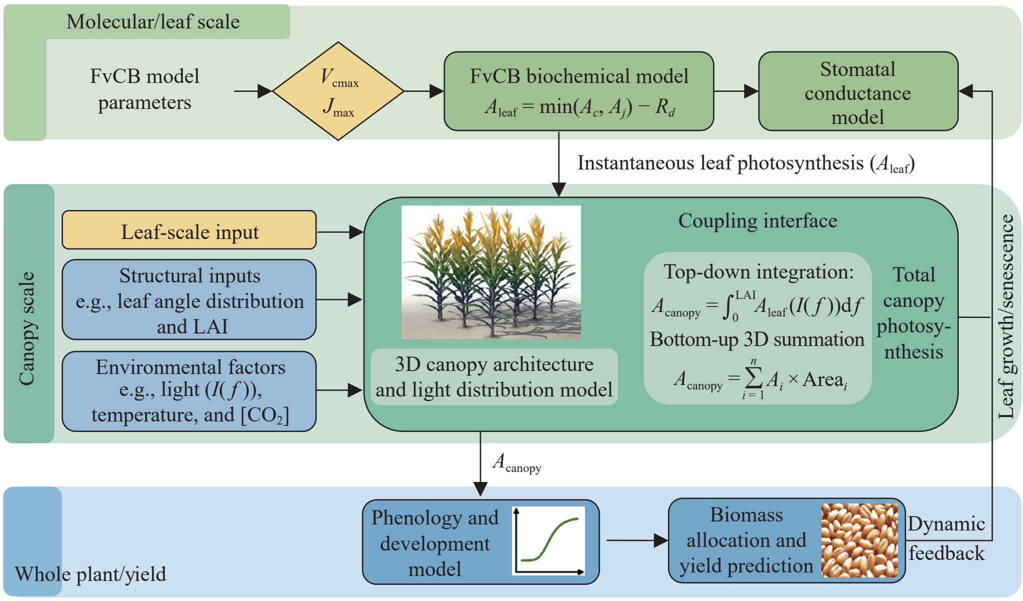

Fig. 1 Multiscale modeling framework linking biochemical to canopy scale.

responses to environmental and physiological attributes and further modeling efforts. Development of the cross-scale modeling framework using the gene-to-phenotype modeling approach can potentially accelerate progress in improving crop resource capture efficiency to support crop improvement through genetic manipulation of photosynthesis.

ACKNOWLEDGMENT

This work was supported by the Natural Science Foundation of Anhui Province of China (No. 2208085MC59) and the Innovation Group Program in Anhui Agricultural University (No. rc312212).

REFERENCES

[1] X. Zhu, S. Long, and D. R. Ort, What is the maximum efficiency with which photosynthesis can convert solar energy into biomass?, *Curr. Opin. Biotechnol.*, 2008, 19(2), 153–159.

[2] M. Reynolds, O. K. Atkin, M. Bennett, M. Cooper, I. C. Dodd, M. J. Foulkes, C. Frohberg, G. Hammer, I. R. Henderson, B. Huang et al., Addressing research bottlenecks to crop productivity, *Trends Plant Sci.*, 2021, 26(6), 607–630.

[3] X. Zhu, S. Long, and D. R. Ort, Improving photosynthetic efficiency for greater yield, *Annu. Rev. Plant Biol.*, 2010, 61, 235–261.

[4] E. A. Ainsworth and S. Long, 30 years of free-air carbon dioxide enrichment (FACE): What have we learned about future crop productivity and its potential for adaptation?, *Global Change Biol.*, 2021, 27(1), 27–49.

[5] S. Long, A. Marshall-Colon, and X. Zhu, Meeting the global food demand of the future by engineering crop photosynthesis and yield potential, *Cell*, 2015, 161(1), 56–66.

[6] D. Leister, Enhancing the light reactions of photosynthesis: Strategies, controversies, and perspectives, *Mol. Plant*, 2023, 16(1), 4–22.

[7] J. R. Evans and T. Lawson, From green to gold: Agricultural revolution for food security, *J. Exp. Bot.*, 2020, 71(7), 2211–2215.

[8] J. L. Araus, R. Sanchez-Bragado, and R. Vicente, Improving crop yield and resilience through optimization of photosynthesis: Panacea or pipe dream?, *J. Exp. Bot.*, 2021, 72(11), 3936–3955.

[9] X. Zhu, Y. Wang, D. R. Ort, and S. Long, e-photosynthesis: A comprehensive dynamic mechanistic model of C3 photosynthesis: From light capture to sucrose synthesis, *Plant, Cell Environ.*, 2013, 36(9), 1711–1727.

[10] Y. Wang, Y. Wang, Y. Tang, and X. Zhu, Stomata conductance as a goalkeeper for increased photosynthetic efficiency, *Curr. Opin. Plant Biol.*, 2022, 70, 102310.

[11] J. R. Evans, Mesophyll conductance: Walls, membranes and spatial complexity, *New Phytol.*, 2021, 229(4), 1864–1876.

[12] R. E. Blankenship and M. Chen, Spectral expansion and antenna reduction can enhance photosynthesis for energy production, *Curr. Opin. Chem. Biol.*, 2013, 17(3), 457–461.

[13] Q. Song, Y. Wang, M. Qu, D. R. Ort, and X. Zhu, The impact of modifying photosystem antenna size on canopy photosynthetic efficiency—Development of a new canopy photosynthesis model scaling from metabolism to canopy level processes, *Plant, Cell Environ.*, 2017, 40(12), 2946–2957.

[14] L. Mao, Q. Song, M. Li, X. Liu, Z. Shi, F. Chen, G. Chen, H. Zheng, and X. Zhu, Decreasing photosystem antenna size by inhibiting chlorophyll synthesis: A double-edged sword for photosynthetic efficiency, *Crop Environ.*, 2023, 2(1), 46–58.

[15] A. P. De Souza, S. J. Burgess, L. Doran, J. Hansen, L. Manukyan, N. Maryn, D. Gotarkar, L. Leonelli, K. K. Niyogi, and S. Long, Soybean photosynthesis and crop yield are improved by accelerating recovery from photoprotection, *Science.*, 2022, 377(6608), 851–854.

[16] J. Kromdijk, K. Głowacka, L. Leonelli, S. T. Gabilly, M. Iwai, K. K. Niyogi, and S. Long, Improving photosynthesis and crop productivity by accelerating recovery from photoprotection, *Science.*, 2016, 354(6314), 857–861.

[17] X. Zhu, D. R. Ort, J. Whitmarsh, and S. Long, The slow reversibility of photosystem II thermal energy dissipation on transfer from high to low light may cause large losses in carbon gain by crop canopies: A theoretical analysis, *J. Exp. Bot.*, 2004, 55(400), 1167–1175.

[18] J. M. McGrath and S. Long, Can the cyanobacterial carbon-concentrating mechanism increase photosynthesis in crop species? A theoretical analysis, *Plant Physiol.*, 2014, 164(4), 2247–2261.

[19] M. Lin, A. Occhialini, P. J. Andralojc, M. A. J. Parry, and M. R. Hanson, A faster rubisco with potential to increase photosynthesis in crops, *Nature*, 2014, 513(7519), 547–550.

[20] X. Zhu, A. R. Portis JR, and S. Long, Would transformation of C3 crop plants with foreign rubisco increase productivity? A computational analysis extrapolating from kinetic properties to canopy photosynthesis, *Plant, Cell Environ.*, 2004, 27(2), 155–165.

[21] S. Long, E. A. Ainsworth, A. D. B. Leakey, J. Nösberger, and D. R. Ort, Food for thought: Lower-than-expected crop yield stimulation with rising CO_2 concentrations, *Science*, 2006, 312(5782), 1918–1921.

[22] E. N. Smith, M. Van Aalst, T. Tosens, Ü. Niinemets, B. Stich, T. Morosinotto, A. Alboresi, T. J. Erb, P. A. Gómez-Coronado, D. Tolleter et al., Improving photosynthetic efficiency toward food security: Strategies, advances, and perspectives, *Mol. Plant*, 2023, 16(10), 1547–1563.

[23] X. Zhu, E. de Sturler, and S. Long, Optimizing the distribution of resources between enzymes of carbon metabolism can dramatically increase photosynthetic rate: A numerical simulation using an evolutionary algorithm, *Plant Physiol.*, 2007, 145(2), 513–526.

[24] B. J. Walker, D. T. Drewry, R. A. Slattery, A. VanLoocke, Y. B. Cho, and D. R. Ort, Chlorophyll can be reduced in crop canopies with little penalty to photosynthesis, *Plant Physiol.*, 2018, 176(2), 1215–1232.

[25] E. A. Cutolo, Z. Guardini, L. Dall'Osto, and R. Bassi, A paler shade of green: Engineering cellular chlorophyll content to enhance photosynthesis in crowded environments, *New Phytol.*, 2023, 239(5), 1567–1583.

[26] X. Zhu, J. P. Lynch, D. S. LeBauer, A. J. Millar, M. Stitt, and S. Long, Plants *in silico*: Why, why now and what?—An integrative platform for plant systems biology research, *Plant, Cell Environ.*, 2016, 39(5), 1049–1057.

[27] T. R. Sinclair, T. W. Rufty, and R. S. Lewis, Increasing photosynthesis: Unlikely solution for world food problem, *Trends Plant Sci.*, 2019, 24(11), 1032–1039.

[28] A. Wu, G. L. Hammer, A. Doherty, S. von Caemmerer, and G. D. Farquhar, Quantifying impacts of enhancing photosynthesis on crop yield, *Nat. Plants*, 2019, 5(4), 380–388.

[29] C. T. de Wit, Photosynthesis of leaf canopies, Tech. Rep. No. 663, Pudoc, Wageningen, Netherlands, 1965.

[30] P. de Reffye, B. Hu, M. Kang, V. Letort, and M. Jaeger, Two decades of research with the GreenLab model in agronomy, *Ann. Bot.*, 2021, 127(3), 281–295.

[31] X. Yin, F. A. Busch, P. C. Struik, and T. D. Sharkey, Evolution of a biochemical model of steady-state photosynthesis, *Plant, Cell Environ.*, 2021, 44(9), 2811–2837.

[32] Y. H. Chew, B. Wenden, A. Flis, V. Mengin, J. Taylor, C. L. Davey, C. Tindal, H. Thomas, H. J. Ougham, P. De Reffye et al., Multiscale digital *Arabidopsis* predicts individual organ and whole-organism growth, *Proc. Natl. Acad. Sci. USA*, 2014, 111(39), E4127–E4136.

[33] G. D. Farquhar, S. von Caemmerer, and J. A. Berry, A biochemical model of photosynthetic CO_2 assimilation in leaves of C3 species, *Planta*, 1980, 149(1), 78–90.

[34] Y. Xiao and X. Zhu, Components of mesophyll resistance and their environmental responses: A theoretical modelling analysis, *Plant, Cell Environ.*, 2017, 40(11), 2729–2742.

[35] A. Garcia, O. Gaju, A. F. Bowerman, S. A. Buck, J. R. Evans, R. T. Furbank, M. Gilliham, A. H. Millar, B. J. Pogson, M. P. Reynolds et al., Enhancing crop yields through improvements in the efficiency of photosynthesis and respiration, *New Phytol.*, 2023, 237(1), 60–77.

[36] Q. Song, F. Liu, H. Bu, and X. Zhu, Quantifying contributions of different factors to canopy photosynthesis in 2 maize varieties: Development of a novel 3D canopy modeling pipeline, *Plant Phenomics*, 2023, 5, 0075.

[37] P. Zhang, S. Xu, G. Zhang, X. Pu, W. Jin, and W. Zhang, Carbon cycle in response to residue management and fertilizer application in a

cotton field in arid Northwest China, *J. Integr. Agric.*, 2019, 18(5), 1103–1119.

[38] P. Boysen Jensen, *The Production of Matter in Agricultural Plants and its Limitation*. Copenhagen, Denmark: Ejnar Munksgaard, 1949.

[39] X. Zhu, M. Hasanuzzaman, A. Jajoo, T. Lawson, R. Lin, C. Liu, L. Liu, Z. Liu, C. Lu, M. Moustakas et al., Improving photosynthesis through multidisciplinary efforts: The next frontier of photosynthesis research, *Front. Plant Sci.*, 2022, 13, 967203.

[40] J. B. Evers, J. Vos, B. Andrieu, and P. C. Struik, Cessation of tillering in spring wheat in relation to light interception and red: Far-red ratio, *Ann. Bot.*, 2006, 97(4), 649–658.

[41] F. J. Bongers, J. B. Evers, N. P. R. Anten, and R. Pierik, From shade avoidance responses to plant performance at vegetation level: Using virtual plant modelling as a tool, *New Phytol.*, 2014, 204(2), 268–272.

[42] J. R. Evans and V. C. Clarke, The nitrogen cost of photosynthesis, *J. Exp. Bot.*, 2019, 70(1), 7–15.

[43] E. Kaiser, A. Morales, and J. Harbinson, Fluctuating light takes crop photosynthesis on a rollercoaster ride, *Plant Physiol.*, 2018, 176(2), 977–989.

[44] W. J. Parton, D. S. Schimel, C. V. Cole, and D. S. Ojima, Analysis of factors controlling soil organic matter levels in Great Plains grasslands, *Soil Sci. Soc. Am. J.*, 1987, 51(5), 1173–1179.

[45] W. J. Parton, J. M. O. Scurlock, D. S. Ojima, T. G. Gilmanov, R. J. Scholes, D. S. Schimel, T. Kirchner, J. C. Menaut, T. Seastedt, E. Garcia Moya et al., Observations and modeling of biomass and soil organic matter dynamics for the grassland biome worldwide, *Global Biogeochem. Cycles*, 1993, 7(4), 785–809.

[46] T. G. Gilmanov, W. J. Parton, and D. S. Ojima, Testing the "CENTURY" ecosystem level model on data sets from eight grassland sites in the former USSR representing a wide climatic/soil gradient, *Ecol. Model.*, 1997, 96(1–3), 191–210.

[47] C. Peng, M. J. Apps, D. T. Price, I. A. Nalder, and D. H. Halliwell, Simulating carbon dynamics along the boreal forest transect case study (BFTCS) in central Canada: 1. Model testing, *Global Biogeochem. Cycles*, 1998, 12(2), 381–392.

[48] W. J. Parton, M. B. Coughenour, J. M. O. Scurlock, D. S. Ojima, T. G. Gilmanov, R. J. Scholes, D. S. Schimel, T. B. Kirchner, J. C. Menaut, T. Seasteadt et al., Global grassland ecosystem modelling: Development and test of ecosystem models for grassland systems, in *Global Change: Effects on Coniferous Forests and Grasslands*. Chichester, England: John Wiley & Sons, 1996, 229–270.

[49] J. M. Melillo, A. D. McGuire, D. W. Kicklighter, B. Moore, C. J. Vorosmarty, and A. L. Schloss, Global climate change and terrestrial net primary production, *Nature*, 1993, 363(6426), 234–240.

[50] J. D. Aber and C. A. Federer, A generalized, lumped-parameter model of photosynthesis, evapotranspiration and net primary production in temperate and boreal forest ecosystems, *Oecologia*, 1992, 92(4), 463–474.

[51] J. A. Foley, I. C. Prentice, N. Ramankutty, S. Levis, D. Pollard, S. Sitch, and A. Haxeltine, An integrated biosphere model of land surface processes, terrestrial carbon balance, and vegetation dynamics, *Global Biogeochem. Cycles*, 1996, 10(4), 603–628.

[52] W. A. Williams, R. S. Loomis, and C. R. Lepley, Vegetative growth of corn as affected by population density. I. Productivity in relation to interception of solar radiation, *Crop Sci.*, 1965, 5(3), 211–215.

[53] J. L. Monteith, Climate and the efficiency of crop production in Britain, *Philos. Trans. R. Soc. Lond. B Biol. Sci.*, 1977, 281(980), 277–294.

[54] M. Monsi, Uber den Lichtfaktor in den Pflanzengesellschaften und seine Bedeutung fur die Stoffproduktion, *J. Japanese Bot.*, 1953, 14, 22–52.

[55] T. R. Sinclair and R. C. Muchow, Radiation use efficiency, *Adva. Agron.*, 1999, 65, 215–265.

[56] T. Sinclair and T. Horie, Leaf nitrogen, photosynthesis, and crop radiation use efficiency: A review, *Crop Sci.*, 1989, 29(1), 90–98.

[57] K. D. Healey, G. L. Hammer, K. G. Rickert, and M. P. Bange, Radiation use efficiency increases when the diffuse component of incident radiation is enhanced under shade, *Aust. J. Agric. Res.*, 1998, 49(4), 665–672.

[58] T. R. Sinclair, T. Shiraiwa, and G. L. Hammer, Variation in crop radiation-use efficiency with increased diffuse radiation, *Crop Sci.*, 1992, 32(5), 1281–1284.

[59] C. J. T. Spitters and A. H. C. M. Schapendonk, Evaluation of breeding strategies for drought tolerance in potato by means of crop growth simulation, *Plant Soil*, 1990, 123(2), 193–203.

[60] R. E. McMurtrie and Y. P. Wang, Mathematical models of the photosynthetic response of tree stands to rising CO_2 concentrations and temperatures, *Plant, Cell Environ.*, 1993, 16(1), 1–13.

[61] S. T. Gower, C. J. Kucharik, and J. M. Norman, Direct and indirect estimation of leaf area index, f_{APAR}, and net primary production of terrestrial ecosystems, *Remote Sens. Environ.*, 1999, 70(1), 29–51.

[62] G. L. Hammer and G. C. Wright, A theoretical analysis of nitrogen and radiation effects on radiation use efficiency in peanut, *Aust. J. Agric. Res.*, 1994, 45(3), 575–589.

[63] J. J. Landsberg and R. H. Waring, A generalised model of forest productivity using simplified concepts of radiation-use efficiency, carbon balance and partitioning, *For. Ecol. Manag.*, 1997, 95(3), 209–228.

[64] P. Zhang, J. Huang, Y. Ma, X. Wang, M. Kang, and Y. Song, Crop/plant modeling supports plant breeding: II. Guidance of functional plant phenotyping for trait discovery, *Plant Phenomics*, 2023, 5, 0091.

[65] P. E. Waggoner and W. E. Reifsnyder, Simulation of the temperature, humidity and evaporation profiles in a leaf canopy, *J. Appl. Meteor. Climatol.*, 1968, 7(3), 400–409.

[66] J. Goudriaan, Crop micrometeorology: A simulation study, PhD dissertation, Wageningen University, Netherlands, 1977.

[67] T. Hirose and M. J. A. Werger, Nitrogen use efficiency in instantaneous and daily photosynthesis of leaves in the canopy of a *Solidago altissima* stand, *Physiol. Plant.*, 1987, 70(2), 215–222.

[68] J. T. Ball, I. E. Woodrow, and J. A. Berry, A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions, in *Progress in Photosynthesis Research*. Dordrecht, Netherlands: Springer, 1987, 221–224.

[69] P. C. Harley, R. B. Thomas, J. F. Reynolds, and B. R. Strain, Modelling photosynthesis of cotton grown in elevated CO_2, *Plant Cell Environ.*, 1992, 15(3), 271–282.

[70] D. Baldocchi, An analytical solution for coupled leaf photosynthesis and stomatal conductance models, *Tree Physiol.*, 1994, 14(7–9), 1069–1079.

[71] P. Sellers, J. A. Berry, G. J. Collatz, C. B. Field, and F. G. Hall, Canopy reflectance, photosynthesis, and transpiration. III. A reanalysis using improved leaf models and a new canopy integration scheme, *Remote Sens. Environ.*, 1992, 42(3), 187–216.

[72] G. D. Farquhar, Models of integrated photosynthesis of cells and leaves, *Philos. Trans. R. Soc. Lond. B Biol. Sci.*, 1989, 323(1216), 357–367.

[73] J. H. M. Thornley, Instantaneous canopy photosynthesis: Analytical expressions for sun and shade leaves based on exponential light decay down the canopy and an acclimated non-rectangular hyperbola for leaf photosynthesis, *Ann. Bot.*, 2002, 89(4), 451–458.

[74] C. Field, Allocating leaf nitrogen for the maximization of carbon gain: Leaf age as a control on the allocation program, *Oecologia*, 1983, 56(2&3), 341–347.

[75] C. Field and H. A. Mooney, Leaf age and seasonal effects on light, water, and nitrogen use efficiency in a California shrub, *Oecologia*, 1983, 56(2&3), 348–355.

[76] J. R. Evans, Photosynthesis and nitrogen relationships in leaves of C3 plants, *Oecologia*, 1989, 78(1), 9–19.

[77] A. D. Friend, A. K. Stevens, R. G. Knox, and M. G. R. Cannell, A process-based, terrestrial biosphere model of ecosystem dynamics (Hybrid v3.0), *Ecol. Model.*, 1997, 95(2&3), 249–287.

[78] A. D. Friend and A. White, Evaluation and analysis of a dynamic terrestrial ecosystem model under preindustrial conditions at the global scale, *Global Biogeochem. Cycles*, 2000, 14(4), 1173–1190.

[79] P. Sands, Modelling canopy production. II. From single-leaf photosynthesis parameters to daily canopy photosynthesis, *Aust. J. Plant Physiol.*, 1995, 22(4), 603–614.

[80] M. Battaglia and P. Sands, Modelling site productivity of *Eucalyptus globulus* in response to climatic and site factors, *Aust. J. Plant Physiol.*, 1998, 24(6), 831–850.

[81] M. U. F. Kirschbaum, CenW, a forest growth model with linked carbon, energy, nutrient and water cycles, *Ecol. Model.*, 1999, 118(1), 17–59.

[82] P. Sellers, D. A. Randall, G. J. Collatz, J. A. Berry, C. B. Field, D. A. Dazlich, C. Zhang, G. D. Collelo, and L. Bounoua, A revised land surface parameterization (SiB2) for atmospheric GCMs. Part I: Model formulation, *J. Climate*, 1996, 9(4), 676–705.

[83] D. G. G. de Pury and G. D. Farquhar, Simple scaling of photosynthesis from leaves to canopies without the errors of big-leaf models, *Plant, Cell Environ.*, 1997, 20(5), 537–557.

[84] L. Gu, D. Baldocchi, S. B. Verma, T. A. Black, T. Vesala, E. M. Falge, and P. R. Dowty, Advantages of diffuse radiation for terrestrial ecosystem productivity, *J. Geophys. Res. Atmos.*, 2002, 107(D6), ACL 2-1–ACL 2-23.

[85] Y. Wang and R. Leuning, A two-leaf model for canopy conductance, photosynthesis and partitioning of available energy I: Model description and comparison with a multi-layered model, *Agric. For. Meteorol.*, 1998, 91(1&2), 89–111.

[86] B. E. Medlyn, R. E. McMurtrie, R. C. Dewar, and M. P. Jeffreys, Soil processes dominate the long-term response of forest net primary productivity to increased temperature and atmospheric CO_2 concentration, *Can. J. For. Res.*, 2000, 30(6), 873–888.

[87] M. U. F. Kirschbaum, D. A. King, H. N. Comins, R. E. Mcmurtrie, B. E. Medlyn, S. Pongracic, D. Murty, H. Keith, R. J. Raison, P. K. Khanna et al., Modelling forest response to increasing CO_2 concentration under nutrient-limited conditions, *Plant, Cell Environ.*, 1994, 17(10), 1081–1099.

[88] R. Leuning, F. M. Kelliher, D. G. G. De Pury, and E. D. Schulze, Leaf nitrogen, photosynthesis, conductance and transpiration: Scaling from leaves to canopies, *Plant, Cell Environ.*, 1995, 18(10), 1183–1200.

[89] D. P. Holzworth, N. I. Huth, P. G. deVoil, E. J. Zurcher, N. I. Herrmann, G. McLean, K. Chenu, E. J. Van Oosterom, V. Snow, C. Murphy et al., APSIM–evolution towards a new generation of agricultural systems simulation, *Environ. Model. Softw.*, 2014, 62, 327–350.

[90] J. W. Jones, G. Hoogenboom, C. H. Porter, K. J. Boote, W. D. Batchelor, L. A. Hunt, P. W. Wilkens, U. Singh, A. J. Gijsman, and J. T. Ritchie, The DSSAT cropping system model, *Eur. J. Agron.*, 2003, 18(3&4), 235–265.

[91] W. G. Duncan, R. S. Loomis, W. A. Williams, and R. Hanau, A model for simulating photosynthesis in plant communities, *Hilgardia*, 1967, 38(4), 181–205.

[92] J. Goudriaan and H. H. Van Laar, Calculation of daily totals of the gross CO_2 assimilation of leaf canopies, *Neth. J. Agric. Sci.*, 1978, 26(4), 373–382.

[93] J. Goudriaan and H. H. Van Laar, *Modelling Potential Crop Growth Processes: Textbook with Exercises*. Dordrecht, Netherlands: Springer, 1994.

[94] X. Yin and H. H. Van Laar, *Crop Systems Dynamics: An Ecophysiological Simulation Model of Genotype-by-Environment Interactions*. Netherland: Wageningen Academic Publishers, 2005.

[95] G. L. Hammer, Z. Dong, G. McLean, A. Doherty, C. Messina, J. Schussler, C. Zinselmeier, S. Paszkiewicz, and M. Cooper, Can changes in canopy and/or root system architecture explain historical maize yield trends in the US corn belt?, *Crop Sci.*, 2009, 49(1), 299–312.

[96] Q. Song, G. Zhang, and X. Zhu, Optimal crop canopy architecture to maximise canopy photosynthetic CO_2 uptake under elevated CO_2-a theoretical study using a mechanistic model of canopy photosynthesis, *Funct. Plant Biol.*, 2013, 40(2), 108–124.

[97] Q. Song, H. Xiao, X. Xiao, and X. Zhu, A new canopy photosynthesis and transpiration measurement system (CAPTS) for canopy gas exchange research, *Agric. For. Meteorol.*, 2016, 217, 101–107.

[98] S. Gu, W. Wen, T. Xu, X. Lu, Z. Yu, X. Guo, and C. Zhao, Use of 3D modeling to refine predictions of canopy light utilization: A comparative study on canopy photosynthesis models with different dimensions, *Front. Plant Sci.*, 2022, 13, 735981.

[99] T. Chang, Z. Shi, H. Zhao, Q. Song, Z. He, J. Van Rie, B. Den Boer, A. Galle, and X. Zhu, 3dCAP-Wheat: An open-source comprehensive computational framework precisely quantifies wheat foliar, nonfoliar, and canopy photosynthesis, *Plant Phenomics*, 2022, 2022, 9758148.

[100] S. Liu, F. Baret, M. Abichou, F. Boudon, S. Thomas, K. Zhao, C. Fournier, B. Andrieu, K. Irfan, M. Hemmerlé et al., Estimating wheat green area index from ground-based LiDAR measurement using a 3D canopy structure model, *Agric. For. Meteorol.*, 2017, 247, 12–20.

[101] S. Liu, P. Martre, S. Buis, M. Abichou, B. Andrieu, and F. Baret, Estimation of plant and canopy architectural traits using the digital plant phenotyping platform, *Plant Physiol.*, 2019, 181(3), 881–890.

[102] X. Yin, J. Harbinson, and P. C. Struik, A model of the generalized stoichiometry of electron transport limited C3 photosynthesis: Development and applications, in *Photosynthesis in Silico: Understanding Complexity from Molecules to Ecosystems*. Dordrecht, Netherlands: Springer, 2009, 247–273.

[103] S. von Caemmerer and R. T. Furbank, Modeling C4 photosynthesis, in *C4 Plant Biology*. San Diego, California: Academic Press, 1999, 173–211.

[104] J. A. Berry and G. D. Farquhar, The CO_2 concentrating function of C4 photosynthesis: A biochemical model, in *Proc. 4th International Congress on Photosynthesis*, London, UK, 1978, 119–131.

[105] G. J. Collatz, M. Ribas-Carbo, and J. A. Berry, Coupled photosynthesis-stomatal conductance model for leaves of C4 plants, *Funct. Plant Biol.*, 1992, 19(5), 519–538.

[106] T. D. Sharkey, Photosynthesis in intact leaves of C3 plants: Physics, physiology and rate limitations, *Bot. Rev.*, 1985, 51(1), 53–105.

[107] Y. Xiao, J. Sloan, C. Hepworth, M. Fradera-soler, A. Mathers, R. Thorley, A. Baillie, H. Jones, T. Chang, X. Chen et al., Defining the scope for altering rice leaf anatomy to improve photosynthesis: A modelling approach, *New Phytol.*, 2023, 237(2), 441–453.

[108] R. A. Boyd, A. Gandin, and A. B. Cousins, Temperature responses of C4 photosynthesis: Biochemical analysis of rubisco, phosphoenolpyruvate carboxylase, and carbonic anhydrase in setaria viridis, *Plant Physiol.*, 2015, 169(3), 1850–1861.

[109] R. F. Sage and D. S. Kubien, The temperature response of C3 and C4 photosynthesis, *Plant Cell Environ.*, 2007, 30(9), 1086–1106.

[110] X. Yin, P. E. L. Van Der Putten, S. M. Driever, and P. C. Struik, Temperature response of bundle-sheath conductance in maize leaves, *J. Exp. Bot.*, 2016, 67(9), 2699–2714.

[111] T. D. Sharkey, What gas exchange data can tell us about photosynthesis, *Plant Cell Environ.*, 2016, 39(6), 1161–1163.

[112] C. Bellasio, D. J. Beerling, and H. Griffiths, Deriving C4 photosynthetic parameters from combined gas exchange and chlorophyll fluorescence using an excel tool: Theory and practice, *Plant, Cell Environ.*, 2016, 39(6), 1164–1179.

[113] X. Yin, M. Van Oijen, and A. H. C. M. Schapendonk, Extension of a biochemical model for the generalized stoichiometry of electron transport limited C3 photosynthesis, *Plant, Cell Environ.*, 2004, 27(10), 1211–1222.

[114] J. Han, Z. Lei, J. Flexas, Y. Zhang, M. Carriquí, W. Zhang, and Y. Zhang, Mesophyll conductance in cotton bracts: Anatomically determined internal CO_2 diffusion constraints on photosynthesis, *J. Exp. Bot.*, 2018, 69(22), 5433–5443.

[115] J. Flexas, M. Barón, J. Bota, J. M. Ducruet, A. Gallé, J. Galmés, M. Jiménez, A. Pou, M. Ribas-Carbó, C. Sajnani et al., Photosynthesis limitations during water stress acclimation and recovery in the drought-adapted *Vitis* hybrid Richter-110 (*V. berlandieri*×*V. rupestris*), *J. Exp. Bot.*, 2009, 60(8), 2361–2377.

[116] R. Leuning, A critical appraisal of a combined stomatal-photosynthesis model for C3 plants, *Plant, Cell Environ.*, 1995, 18(4), 339–355.

[117] S. Li, D. H. Fleisher, Z. Wang, J. Barnaby, D. Timlin, and V. R. Reddy, Application of a coupled model of photosynthesis, stomatal conductance and transpiration for rice leaves and canopy, *Comput. Electron. Agric.*, 2021, 182, 106047.

[118] R. M. Deans, T. J. Brodribb, F. A. Busch, and G. D. Farquhar, Optimization can provide the fundamental link between leaf photosynthesis, gas exchange and water relations, *Nat. Plants*, 2020, 6(9), 1116–1125.

[119] X. Yin and P. C. Struik, Can increased leaf photosynthesis be converted into higher crop mass production? A simulation study for rice using the crop model GECROS, *J. Exp. Bot.*, 2017, 68(9), 2345–2360.

[120] J. Harbinson and X. Yin, Modelling the impact of improved

photosynthetic properties on crop performance in Europe, *Food Energy Secur.*, 2023, 12(1), e402.

[121] X. Zhu, Q. Song, and D. R. Ort, Elements of a dynamic systems model of canopy photosynthesis, *Curr. Opin. Plant Biol.*, 2012, 15(3), 237–244.

[122] V. Letort, P. Mahe, P. H. Cournede, P. de Reffye, and B. Courtois, Quantitative genetics and functional-structural plant growth models: Simulation of quantitative trait loci detection for model parameters and application to potential yield optimization, *Ann. Bot.*, 2008, 101(8), 1243–1254.

[123] V. Picheny, P. Casadebaig, R. Trépos, R. Faivre, D. Da Silva, P. Vincourt, and E. Costes, Using numerical plant models and phenotypic correlation space to design achievable ideotypes, *Plant, Cell Environ.*, 2017, 40(9), 1926–1939.

[124] M. Rakocevic, R. V. Ribeiro, P. E. Ribeiro Marchiori, H. F. Filizola, and E. R. Batista, Structural and functional changes in coffee trees after 4 years under free air CO_2 enrichment, *Ann. Bot.*, 2018, 121(5), 1065–1078.

[125] Q. Song, V. Srinivasan, S. Long, and X. Zhu, Decomposition analysis on soybean productivity increase under elevated CO_2 using 3D canopy model reveals synergestic effects of CO_2 and light in photosynthesis, *Ann. Bot.*, 2020, 126(4), 601–614.

[126] X. Yin and P. C. Struik, Applying modelling experiences from the past to shape crop systems biology: The need to converge crop physiology and functional genomics, *New Phytol.*, 2008, 179(3), 629–642.

[127] J. Gu, X. Yin, T. J. Stomph, and P. C. Struik, Can exploiting natural genetic variation in leaf photosynthesis contribute to increasing rice productivity? A simulation analysis, *Plant, Cell Environ.*, 2014, 37(1), 22–34.

[128] X. Yin and P. C. Struik, Constraints to the potential efficiency of converting solar radiation into phytoenergy in annual crops: From leaf biochemistry to canopy physiology and crop ecology, *J. Exp. Bot.*, 2015, 66(21), 6535–6549.

[129] A. Wu, J. Brider, F. A. Busch, M. Chen, K. Chenu, V. C. Clarke, B. Collins, M. Ermakova, J. R. Evans, G. D. Farquhar et al., A cross-scale analysis to understand and quantify the effects of photosynthetic enhancement on crop growth and yield across environments, *Plant Cell Environ.*, 2023, 46(1), 23–44.

[130] P. Zhang, X. Wang, J. Huang, Y. Zhang, Z. Zhang, Y. Yu, P. de Reffye, M. Kang, and Y. Song, Extension of the GreenLab in modelling maize canopy photosynthesis under high plant densities for trait discovery, *Field Crops Res.*, 2025, 334, 110155.

Pengpeng Zhang received the BS degree in crop cultivation and farming system from Shihezi University, Shihezi, China, in 2017, and the PhD degree in crop physiology and modeling from Anhui Agricultural University, Hefei, China, in 2024. He is currently a postdoctoral fellow at Institute for Crop Sciences, Chinese Academy of Agricultural Sciences, China. His research interests include modelling and optimization of crop canopy photosynthesis and industrial internet.

Youhong Song received the BS and PhD degrees in crop physiology and modeling from China Agricultural University, Beijing, China, in 2000 and 2003, respectively, and the PhD degree in crop biology from University of Newcastle, Newcastle, Australia, in 2012. He is currently a professor at School of Agricultural Sciences, Jiangxi Agricultural University, China, and an adjunct principal fellow at Centre for Crop Science, Queensland Alliance for Agriculture and Food Innovation, The University of Queensland, Australia. He has published more than 100 papers in refereed journals. He is the associate editor of *Crop and Pasture Science*, editorial board member of *npj Sustainable Agriculture*, and guest editor of *European Journal of Agronomy*. His research interests include crop physiology, agronomy, biology, and crop modelling applies, extending from molecular to whole plant level.