Validation of Spring Wheat Responses to Elevated CO₂, Irrigation, and Nitrogen Fertilization in the Community Land Model 4.5

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Abstract The Community Land Model (CLM) started to incorporate crop growth models since version 4.0 in 2012. Since then, the crop model in CLM has been evolved remarkably, but some of the key crop growth responses to environmental conditions (such as the elevated CO₂) have not been well validated. Here, we set up single point simulations with CLM (version 4.5) and validated spring wheat growth response against the Maricopa spring wheat Free Air CO₂ Enrichment (FACE) experiment that consisted of multiyear paired treatments to understand the growth response to elevated CO₂, irrigation, nitrogen fertilization, and their interactions. Overall, CLM showed too positive growth response to elevated CO₂ but insufficient growth response to irrigation. The overestimated growth response to elevated CO₂ may be due to ignoring factors (e.g., leaf traits) that will limit crop growth under elevated CO₂. The insufficient response to irrigation is due to CLM simulating lower latent heat flux during April and May, which resulted in higher soil moisture. In response to nitrogen fertilization, CLM underestimated leaf area index increase but overestimated grain yield increase. In terms of energy fluxes, CLM showed decreased latent heat flux in response to elevated CO₂ but increased latent heat flux in response to nitrogen fertilization, but the response magnitude was much smaller than the observations. Based on these validations, we summarized further model developments for CLM to better simulate crop growth process.

1. Introduction

The Community Land Model (CLM) (Oleson et al., 2013) is a state-of-the-art land surface model that simulates biogeochemical (radiation transfer, vegetation-soil-hydrology, surface energy fluxes, etc.) and biogeophysical (soil carbon and nitrogen cycle, vegetation photosynthesis, dynamic vegetation growth, etc.) processes. A CLM grid includes a subset of land units and vegetation functional types, as well as multiple layers of snow and soil. CLM is the default land model in the Community Earth System Model (Hurrell et al., 2015), and can be run either online coupled with the rest of Community Earth System Model (atmosphere and ocean) or offline (land model only, forced with climate datasets) for multiple spatial extents (site, regional, and global) and different resolutions. It has been recognized as one of the leading land surface models internationally and has been also used in other regional modeling systems, such as WRF-CLM (Lu et al., 2015; Subin et al., 2011), RegCM-CLM (Li et al., 2015; Steiner et al., 2009), and COSMO-CLM (Roeckel & Geyer, 2008). Levis et al. (2012) first added crop growth modules from the AgroIBIS model (Kucharik, 2003); since then CLM has been expanded to represent more crops types and processes, such as soybean nitrogen fixation (Drewniak et al., 2013), ozone impacts on yield (Lombardozzi et al., 2015), winter wheat growth response to cold hazards (Lu et al., 2017). CLM simulates nine crop types, which accounts for 54% of the global total crop production (other production is represented by the most similar resolved crop type): maize, soybean, spring wheat, winter wheat, cotton, rice, sugarcane, tropical maize, and tropical soybean.

One urgent requirement for CLM crop model is to add more validations on the key crop growth responses to environmental conditions, such as crop growth response to elevated CO₂, irrigation, and nitrogen fertilizations. Crop yields are greatly sensitive to irrigation and fertilizer usage (Mueller et al., 2013), and the rising CO₂ concentrations could have multiple effects on crop growth. Elevated CO₂ increases the CO₂
concentrations at the surface of leaves, which causes smaller opening of stomata and somewhat restricts the conduction of CO₂ to participate in photosynthesis (Drake et al., 1997). The smaller stomatal conductance also restricts evapotranspiration, which allows plants to conserve more water (or grow more with the same amount of water). As evapotranspiration decreases, it also increases leaf temperature and the partial pressure of water vapor inside the leaves, which increases leaf transpiration (Kimball et al., 1995). Elevated CO₂ effects are also related to limitations on other resources for growth. The stimulation of photosynthesis by elevated CO₂ can be much smaller when nitrogen is limiting. Therefore, the elevated CO₂ interaction with irrigation and fertilization exerts large uncertainties on crop growth. Validations on crop growth response to elevated CO₂ for crop models that used for future food projection are especially important to understand the uncertainties. Along the long history of development of other crop models, many other crop models have validated their crop growth response to land managements and elevated CO₂ using data from Free Air CO₂ Enrichment (FACE) experiments.

FACE experiment (FACE) is one of the most realistic observations in studying the crop growth response to elevated CO₂. The FACE facility ejects CO₂ at the desired amount into the open field throughout the growing season, and crops in the open field are still receiving the natural weather and utilizing the soil water and nutrient without the boundary limits, unlike in enclosure experiments. FACE facility was first established by Brookhaven National Laboratory (Lewin et al., 1992) and tested at the field of Maricopa Agricultural Center of the University of Arizona for cotton and then applied for other crops at Maricopa (spring wheat, sorghum) and other sites as well. There are also several issues with the FACE experiments, such as the blower (used to mixing the CO₂ and surrounding air), which could result warm night temperature (Pinter et al., 1992; Okada et al., 2001) have abandoned blowers and instead adopted pressure and tubes with numerous holes to mix CO₂ and surrounding air.

Among the many FACE sites, Maricopa spring wheat FACE site (1992–1997) is one of the most widely used sites for the crop model validations (Kimball et al., 2017). The site not only looked at the crop growth response to elevated CO₂ but also focused on the response to elevated CO₂ interaction with high and low levels of irrigation and nitrogen fertilization. DEMETER is the first model used the Maricopa spring wheat FACE site observations to validate its crop growth response to elevated CO₂ (Grossman et al., 1995; Kartschall et al., 1995), following ecosys (Grant et al., 1995, 1999), CERES-wheat (Tubiello et al., 1999), AFRCWHEAT2 (Ewert et al., 2002; Jamieson et al., 2000), FASSET (Jamieson et al., 2000), LINTULCC2 (Ewert et al., 2002), Sirius (Ewert et al., 2002; Jamieson et al., 2000), APSIM-Wheat (Asseng et al., 2004), RZWQM2-CERES-Wheat4.0 (Ko et al., 2010), and GECROS (Yin & Struik, 2010). These models vary in their complexity in simulations on photosynthesis and respiration. Some crop models used RUE empirical function, where elevated CO₂ impact on maximum photosynthesis could be predetermined and calibrated. Some crop models used the biochemical photosynthesis function coupled with stomatal function, in which photosynthesis and stomatal conductance are interrelated and require iteration to get the equilibrium solution.

CLM uses biochemical photosynthesis models for C3 (Farquhar et al., 1980) and C4 (Collatz et al., 1992) plants, with modifications described in Bonan et al. (2011). C3 plants’ photosynthesis are colimited by RuBP carboxylase (Rubisco) limited rate of carboxylation (Ac), the light-limited rate of carboxylation (Aj), and the product-limited rate of carboxylation (Ap). Ac and Aj largely depend on the internal leaf CO₂ partial pressure (Ci), which was directly affected by the elevated atmospheric CO₂. A Ball-Berry type stomatal conductance model (Collatz et al., 1991) was coupled with the photosynthesis models, where elevated atmospheric CO₂ directly affects the leaf surface CO₂ partial pressure (Cs). Then, photosynthesis and stomatal resistance are interdependent, where reduced stomatal resistance could increase photosynthesis and then
more water evaporated, which in turn can dry the soil and result in an increase of stomatal resistance and reduced photosynthesis.

Water limitation in CLM is through a plant water stress indicator ($\beta_t$). $\beta_t$ varies between 0 and 1, where 0 indicates fully water stress and 1 indicates no water stress. $\beta_t$ at each soil layer is a function of soil water potential and root fraction. Total soil column $\beta_t$ is calculated by aggregating $\beta_t$ at each soil layer. $\beta_t$ directly controls photosynthesis and stomatal conductance. $\beta_t$ scales the intercept in the Ball-Berry stomatal equation; when $\beta_t$ is low, then the stomatal conductance will be low. The parameters used in Farquhar ($v_{cmax}$ and $j_{max}$) are scaled with $\beta_t$ as well. Unlike many other crop models, which use a water stress factor to scale biomass or crop growth, in CLM, water stress affects crop growth through directly altering photosynthesis and stomatal conductance.

Nitrogen limitation in CLM4.5 is through the down regulation of potential photosynthesis without considering the nitrogen demand and supply. Photosynthesis is calculated from a potential photosynthesis at the particular CO$_2$, water supply, and radiation available, but without a limiting nitrogen supply. Then, the complex underground biogeochemical processes will determine the nitrogen demand and supply. When the nitrogen demand is higher than nitrogen supply, then the potential photosynthesis will be reduced by the limitation factor. The plant accessible soil nitrogen pool is the soil mineral nitrogen pool, which can be increased by fertilization. As the nitrogen is allocated to plant tissues, the soil mineral nitrogen pool is reduced. The biogeochemical model also accounts for atmospheric nitrogen deposition and biological fixation, as well as nitrogen losses due to denitrification and leaching.

Although CLM considered vegetation growth response to elevated CO$_2$, water and nutrient stress, the crop growth response to these environmental conditions has never been validated, especially against FACE experiment. The objective of our study is to validate CLM crop growth response to elevated CO$_2$, irrigation, and nitrogen fertilization against field measurements and summarize further model developments for CLM to better simulate crop growth process.

2. Methods

2.1. Spring wheat-FACE experiment at Maricopa

The Maricopa spring wheat FACE experiment was conducted during four growing seasons, with two seasons (1992–1994) focused on crop growth response to elevated CO$_2$ at two levels of irrigation (given moderate nitrogen fertilization) and two seasons (1995–1997) focused on crop growth response to elevated CO$_2$ at two levels of nitrogen fertilization (given moderate irrigation). In the FACE field, there were four replicated 25-m diameter circular plots. The FACE plots were equipped with 2.5-m tall vertical pipes around the plots that ejected concentrated CO$_2$-enriched air into the plots at controlled rates to maintain the desired CO$_2$ concentrations in the plots. The CO$_2$ concentrations at the center of the FACE plots were maintained at 550 ppm during 1992–1994, whereas they were enriched by 200 ppm above the ambient (360 ppm) during the 1995–1997 experiments. There were four corresponding control plots at ambient CO$_2$. Each circular plot was divided into two semicircular halves with each half receiving one of two levels of irrigation or of two levels of nitrogen fertilization (Table 1). Spring wheat was planted in December and harvested in May. The site used a drip irrigation system, which not only applied irrigation but also applied nitrogen fertilizer in the irrigation water. Irrigation in 1993 was higher than 1994, because a large amount of irrigation (317 mm) was applied into both the low-irr and high-irr treatments before planting in order to achieve good germination. In subsequent years, a portable sprinkler irrigation was installed for a short time at the beginning of the seasons to achieve good germination, and it required less water than using the subsurface drip system for germination. The site had weekly or biweekly measurements of crop growth (e.g., LAI [leaf area index] and tissue biomass) and hourly or 15-min microclimate measurements (e.g., soil moisture and radiation) (Kimball et al., 2017).

2.2. CLM4.5 Simulations

We performed site simulations with CLM4.5 for the 16 treatments, forcing with the site observed hourly meteorology (wind, downward solar radiation, precipitation, air temperature and dew point air temperature). We applied the same amounts of irrigation water and nitrogen fertilizer as in the experiments, which were evenly distributed across the same days as in the experiments. We chose a CLM compset BGCCROP for
all the simulations, which allows a dynamic below ground biogeochemical process and dynamic crop growth. Such a compset also requires long-term spin-up for the soil carbon pools to reach steady states (Shi et al., 2013). Therefore, we repeatedly used the 1993–1996 input data and ran simulations for 500 hundred years for the spin-up. We calibrated crop growth related parameters for one treatment (ambient CO2; ample water and N), and then we applied the calibrated parameters to other treatments. It is important that all the simulations used the same parameters because the differences between two simulations are only due to the differences in CO2, irrigation, or nitrogen fertilization.

2.3. Calibration at Treatment 902

Treatment 902 was well irrigated with ample nitrogen fertilization under ambient CO2. We chose the treatment 902 for calibration because it represents a normal case with an unstressed crop. The calibration involved three steps. The first step was to calibrate parameters that control phenology. CLM simulates four phenology phases, including planting, leaf emergence, grain fill, and harvest. The minimum and maximum planting date determines the desired planting window. Crops will not be planted if the dates do not reach the minimum planting date but could be planted if the dates exceed the maximum planting date. When the time falls between min and max planting date, there are three conditions that need to be satisfied: (1) 10-day average air temperature greater than 280.15 K, (2) 10-day average minimum temperature greater than 272.15 K, (3) 20-year running mean growing degree days from April to September greater than 50 degree-days. The original spring wheat (which does not have a vernalization requirement) planting window was set between 1 April and 15 June in the Northern Hemisphere, whereas at Maricopa and other locations like Mexico that are closer to the equator than the winter wheat (which requires vernalization) belt, spring wheat is normally planted in December in the Northern Hemisphere. Therefore, we modified the planting window to 5–25 December. The planting actually occurred at the first day as the simulation started at 17 December. The observed planting date was 15 December. The hourly data we obtained started at 17 December but only 2 days bias is acceptable for the phenology. We did not change parameters for temperature because they were met already. Once the planting date was determined, we needed to determine the growing degree days for maturity (GDDm). Growing degree days is the key variable controlling phenology, and is defined as heat accumulation during the whole growing season or over a certain period. It was calculated by accumulating the difference (no accumulation if less than 0) between the target temperature (e.g., mean daily air temperature) and base temperature and normally has a maximum daily increment. CLM has different GDD thresholds to determine if crop growth should enter the next phenology phase. GDDm is the threshold that determines whether the crop should be harvested, and the other thresholds for leaf emergence and grain fill are fractions of GDDm. Thus, GDDm should be the first one to be determined. We changed GDDm from 1700 to 1900 with a resultant maturity date of 14 May. The observed maturity date was 13 May. After determining GDDm, then the two parameters that determine when to enter leaf emergence (lfemerg) and grain

| Treatment # | Years      | Irrigation (mm) | Nitrogen (gN/m²) | CO₂ (ppm) |
|-------------|------------|-----------------|------------------|-----------|
| 901         | 1992–1993  | 592             | 27.7             | 360       |
| 902         | 1992–1993  | 919             | 27.7             | 360       |
| 903         | 1992–1993  | 592             | 27.7             | 550       |
| 904         | 1992–1993  | 919             | 27.7             | 550       |
| 905         | 1993–1994  | 287             | 26.1             | 360       |
| 906         | 1993–1994  | 629             | 26.1             | 360       |
| 907         | 1993–1994  | 287             | 26.1             | 550       |
| 908         | 1993–1994  | 629             | 26.1             | 550       |
| 909         | 1995–1996  | 592             | 9.97             | 360       |
| 910         | 1995–1996  | 653             | 38.29            | 360       |
| 911         | 1995–1996  | 592             | 9.97             | 560       |
| 912         | 1995–1996  | 653             | 38.29            | 560       |
| 913         | 1996–1997  | 548             | 5.3              | 360       |
| 914         | 1996–1997  | 621             | 39.3             | 360       |
| 915         | 1996–1997  | 548             | 5.3              | 560       |
| 916         | 1996–1997  | 621             | 39.3             | 560       |
Leaf carbon keeps increasing until LAI reaches the maximum, during the grain fill phase, carbon allocation mainly to grain, and a small fraction to stem and root. Here, we only calibrated carbon allocation parameters that determine how much of the available carbon was allocated to different tissues, while not calibrating the parameters involved in photosynthesis and respiration. Three carbon allocation parameters are modified based on sensitivity tests, including arooti, bfact, and astemf. These parameters do not have physical meanings but were just used to adjust the carbon allocation algorithm.

After the modifications of the phenology and carbon allocation parameters (Table 2), we noticed the LAI decline was still not well matched to observation due to the slow senescence rate. Therefore, we adjusted leaf longevity from 1 year to 3 months to accelerate the leaf senescence during grain decline was still not well matched to observation due to the slow senescence rate. Therefore, we adjusted leaf longevity from 1 year to 3 months to accelerate the leaf senescence during grain fill, and we also reduced the maximum canopy height to 0.9 to better match the observations (Table 2).

3. Results

3.1. Crop Growth in Calibration and Validation

The calibration using treatment 902 largely improved the simulation on crop growth and phenology. The simulated planting, anthesis, and maturity dates were within 2 days of the observations. However, there were several problems in simulating leaf, stem, above-ground biomass, and grain growth that could not be resolved by the calibration. During the vegetative phase, the simulated LAI and leaf weight never decreased (Figures 1a and 1b) because leaf senescence occurs only after the grain fill phase in CLM has started. The observations from treatment 902 suggest there was a decrease in LAI and leaf weight near anthesis, which has been attributed to delays in processing (P.J. Pinter, Jr. personal communication). Unfortunately, during this first year, personnel were overwhelmed by the rapid increase in volume of samples, and there was some deterioration of leaf area before the samples could be processed. The large sample volume was expected and mediated in subsequent years. During the grain fill phase, the simulated stem weight (Figure 1d) was not decreased because there is no stem senescence scheme in CLM. Another problem for stem is that the stem area index (Figure 1c) in CLM was calculated in proportion to LAI and not related to the stem weight. The grain weight (Figure 2e) showed a similar increase at the beginning of grain fill stage, but the grain yield was lower by 88.3 g/m² due to the slowing of grain weight increase as maturity approached. Such slowing of grain weight accumulation was not always shown for the other treatments due to contributions from other errors in CLM (e.g., higher LAI, higher soil moisture, or higher nutrient), which led to higher grain weight. The above-ground biomass (Figure 1f) was well simulated during the vegetative phase, but when entered the grain fill phase, is was underestimated, which was due to the above-ground biomass in CLM only including leaf, stem, and grain, and not chaff weight.

The validation of the other 15 treatments showed 12% lower $R^2$ and 36% higher Root Mean Square Error (RMSE) than calibration treatment 902 on average across leaf, stem, grain, and above-ground biomass simulations (Table 3). Many of the errors were due to CLM not simulating phenology variations well enough across the different treatments. The observed anthesis dates varied from 19 March (910) to 4 April (916),
while the simulated anthesis dates showed only 3 days (24 March to 27 March) difference (Table 4). The observed physiological maturity date showed a similar large variation (19 days), which was not seen in CLM simulations (only 4-day variation). The planting date simulations were fine. The 1–2-day late planting in CLM was due to the hourly meteorology forcing data only available 1 or 2 days later than the observed planting date.

Another problem that largely affected the LAI simulation is that CLM adopted a fixed specific leaf area (SLA) parameter throughout the growing season. The SLA used in CLM for spring wheat is 0.07 m²/gC, equivalent to 0.028 m²/gLeaf weight, assuming the leaf carbon content is 40% of leaf weight. But the observed SLA showed large variation during the growing season, and the values of SLA were different across treatments. Treatments 901–904 showed high SLA at the beginning and then declined during anthesis and finally increased. Treatments 913–916 showed gradual increasing. LAI is equal to leaf weight multiplied by SLA. The fixed SLA in CLM resulted a poor LAI simulation even with a reasonable leaf weight simulation for those treatments that the fixed SLA used in CLM was far away from the observations. For example, for 913–916, the averaged SLA was 0.02 m²/gLeaf weight. The simulated LAI was consistently overestimated (40% higher averaged across 913–916) even with good leaf weight simulations (0.1% lower than observation averaged across 913–916). In terms of elevated CO₂ impact on SLA, while some other observations found

FIGURE 1. Seasonal variation of (a) leaf area index (LAI; m²/m²), (b) leaf weight (g/m²), (c) stem area index (SAI; m²/m²), (d) stem weight (g/m²), (e) grain weight (g/m²), and (f) above-ground biomass (g/m²) at treatment 902.

FIGURE 2. Percentage responses of seasonal mean leaf area index, leaf weight, stem weight, grain weight, and above ground biomass weight to (a) elevated CO₂, (b) water limitation, and (c) nitrogen limitation.
elevated CO2 could result a lower SLA (Ainsworth et al., 2002; Yin, 2002), we found no statistically significant difference between the paired ambient and elevated CO2 treatments in the observed periods.

We also found a problem in the carbon allocation with the validations. For some treatments with elevated CO2, LAI was stimulated to the maximum allowance. When that happens, all the available carbon will be applied to root. Leaf, stem, and above-ground weight stays the same at the time when LAI reaches the maximum. Such an approach can result in an underestimation of stem and above-ground weight and overestimation of root carbon. On average, CLM underestimated above-ground biomass by 7% (117 g/m2) and overestimated grain yield by 13% (91 g/m2) (Table 4).

### 3.2. Crop Growth Responses to CO2, Irrigation, and N Fertilization

CLM spring wheat leaf growth showed a much higher response to elevated CO2 than the observations but insufficient responses to irrigation and N fertilization (Figure 2). In response to elevated CO2, the simulated seasonal mean LAI and leaf weight both increased by 27.7% averaged across the eight-paired treatments, while the observed seasonal mean LAI actually decreased by 0.6% and leaf weight decreased by 2.2% (Figure 2a). The LAI for the ambient treatments (2.5 m2/m2 in average) was quite similar to the observations (2.6 m2/m2 in average). For the FACE treatments, simulated LAI was 3.2 m2/m2, but observed was only 2.5 m2/m2. Even though the average observed LAI was reduced, elevated CO2 did stimulate leaf growth during the early growing season, but the accelerated leaf senescence during the grain fill stage canceled the stimulation at the early growing season and therefore resulted in a reduced LAI. The observed leaf growth at low irrigation treatments was 28.4% lower for LAI and 25.6% lower for leaf weight compared to the ample irrigation, whereas the simulated LAI and leaf weight values were reduced by 6.7%, but such decreases in CLM were actually only shown in 1993–1994 (Figure 2b). The CLM crop growth during 1992–1993 was not affected by irrigation, which will be discussed later. The lower amount of nitrogen fertilization reduced observed LAI and leaf weight by 36.5% and 31.2%. CLM also showed reduced LAI and leaf weight by 21.6%, but still slightly smaller than observation (Figure 2c).

### Table 3

The $R^2$ and Root Mean Square Error (RMSE) between observation and simulation for the calibration treatment 902, and the average $R^2$ and RMSE for the other validation treatments (901,903-916)

|         | LAI | SAI | Leaf weight | Stem weight | Grain weight | Above-ground biomass |
|---------|-----|-----|-------------|-------------|--------------|---------------------|
| $R^2$   |     |     |             |             |              |                     |
| Calibration | 0.78 | 0.88 | 0.94        | 0.97        | 0.96         | 0.98                |
| Validation | 0.67 | 0.71 | 0.75        | 0.86        | 0.92         | 0.92                |
| RMSE    |     |     |             |             |              |                     |
| Calibration | 1.03 | 0.30 | 258.74      | 1,022.55    | 488.73       | 1,852.92            |
| Validation | 1.63 | 0.32 | 465.52      | 1,237.23    | 575.13       | 2,471.23            |

### Table 4

Observed and Simulated Phenology, Dry Matter, and Harvest Index for the 16 Treatments

| Planting | Anthesis | Physiological maturity | Above-ground DM (g/m$^2$) | Grain yield (g/m$^2$) | Harvest index |
|----------|----------|------------------------|---------------------------|-----------------------|---------------|
| Obs      | CLM      | Obs                    | CLM                       | Obs                   | CLM           |
| 901      | 15 Dec   | 17 Dec                 | 25 Mar                    | 26 Mar                | 6 May         | 14 May        | 1,491.30     | 1,586.10     | 595.40       | 740.81       | 0.40          | 0.47          |
| 902      | 15 Dec   | 17 Dec                 | 26 Mar                    | 26 Mar                | 13 May        | 14 May        | 1,827.60     | 1,614.75     | 836.90       | 748.63       | 0.46          | 0.46          |
| 903      | 15 Dec   | 17 Dec                 | 22 Mar                    | 27 Mar                | 4 May         | 15 May        | 1,552.30     | 1,540.79     | 719.70       | 961.68       | 0.46          | 0.62          |
| 904      | 15 Dec   | 17 Dec                 | 24 Mar                    | 26 Mar                | 6 May         | 15 May        | 1,983.20     | 1,543.38     | 903.50       | 964.25       | 0.46          | 0.62          |
| 905      | 7 Dec    | 8 Dec                  | 6 Apr                    | 27 Mar                | 21 May        | 14 May        | 1,385.80     | 1,339.92     | 474.40       | 686.30       | 0.34          | 0.51          |
| 906      | 7 Dec    | 8 Dec                  | 6 Apr                    | 27 Mar                | 10 May        | 14 May        | 1,800.00     | 1,549.99     | 743.50       | 727.58       | 0.41          | 0.47          |
| 907      | 7 Dec    | 8 Dec                  | 1 Apr                    | 27 Mar                | 10 May        | 14 May        | 1,583.00     | 1,620.58     | 591.80       | 956.83       | 0.37          | 0.59          |
| 908      | 7 Dec    | 8 Dec                  | 2 Apr                    | 28 Mar                | 17 May        | 14 May        | 1,927.70     | 1,487.83     | 831.10       | 923.53       | 0.43          | 0.62          |
| 909      | 15 Dec   | 16 Dec                 | 28 Mar                    | 24 Mar                | 3 May         | 12 May        | 1,262.80     | 1,410.52     | 577.20       | 657.47       | 0.46          | 0.47          |
| 910      | 15 Dec   | 16 Dec                 | 29 Mar                    | 24 Mar                | 10 May        | 12 May        | 1,681.80     | 1,410.70     | 739.90       | 657.65       | 0.44          | 0.47          |
| 911      | 15 Dec   | 16 Dec                 | 27 Mar                    | 25 Mar                | 3 May         | 13 May        | 1,415.90     | 1,480.43     | 645.70       | 700.78       | 0.46          | 0.47          |
| 912      | 15 Dec   | 16 Dec                 | 26 Mar                    | 25 Mar                | 10 May        | 13 May        | 1,611.50     | 1,624.54     | 849.40       | 942.84       | 0.53          | 0.58          |
| 913      | 15 Dec   | 16 Dec                 | 2 Apr                     | 24 Mar                | 8 May         | 11 May        | 1,265.80     | 807.14       | 504.30       | 465.50       | 0.40          | 0.58          |
| 914      | 15 Dec   | 16 Dec                 | 3 Apr                     | 25 Mar                | 9 May         | 13 May        | 1,269.70     | 1,378.81     | 612.60       | 664.95       | 0.48          | 0.48          |
| 915      | 15 Dec   | 16 Dec                 | 1 Apr                     | 25 Mar                | 8 May         | 11 May        | 1,203.70     | 811.17       | 530.60       | 447.48       | 0.44          | 0.55          |
| 916      | 15 Dec   | 16 Dec                 | 4 Apr                     | 27 Mar                | 10 May        | 14 May        | 1,399.80     | 1,486.85     | 715.70       | 910.80       | 0.51          | 0.61          |

*Anthesis is a part of the vegetative stage and not specifically simulated in CLM, so we calculated the anthesis date as 7 days before the vegetative phase end.*

*Physiological maturity date was the date at the end of grain fill stage.*

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Unlike the overall reduced leaf growth, the observed stem growth was largely stimulated (17.9%) by elevated CO2, while the simulated stem weight was decreased by 8.8% at elevated CO2 due to the previously mentioned phenology error in CLM (Figure 2a). The water limitation decreased observed stem weight by 15.6%, but the CLM-simulated decrease was only 2.0% in CLM (Figure 2b). Unlike the largely decreased leaf growth, nitrogen limitation actually did not decrease stem growth in observation, where stem weight increased by 0.8%. CLM showed decreased stem weight (21.7%) under the nitrogen limitation (Figure 2c).

CLM underestimated the mean grain weight response to CO2 and irrigation, while overestimating the response to the nitrogen limitation. CLM simulated the mean grain weight responses to elevated CO2, irrigation, and N fertilization were 27.8%, 0.3%, and −20.4%, while the observed responses were 30.9%, 4.7%, and −6.7% respectively.

The responses of above-ground biomass are the combined responses from leaf, stem, and grain. CLM underestimated above-ground biomass responses to CO2 and water limitation, while overestimating the response to nitrogen limitation. CLM simulated above-ground biomass responses to elevated CO2, water limitation, and nitrogen limitation were 6.7%, −3.0%, and −21.9%, while the observed responses were 16.6%, −10.6%, and −8.2%, respectively.

The observations showed opposite tendencies of the crops to allocate the extra CO2 and nitrogen resources between leaf and stem. Elevated CO2 only slightly increased leaf growth but greatly increased stem growth, while N fertilization greatly increased leaf weight but only slightly increased stem weight. CLM simulations did not exhibit such tendencies at all because carbon allocations between leaf and stem only depends on growing degree days and a set of predefined parameters, and there is no response to environmental stress.

### 3.3. Energy Flux Responses to Elevated CO2 and N Fertilization

Net radiation and ground heat flux simulations are well matched the observations (Table 5). CLM4.5 slightly underestimated the net radiation and ground heat flux by 4.3 and 0.02 W/m², which are 3% and 1% lower than the observation, respectively. However, the simulated energy partitioning between sensible heat (SH) and latent heat (LH) fluxes did not agree with the observations. The simulated LH is 41.3 W/m² (32%) lower than observed, and simulated SH is 37.8 W/m² (1517%) higher than observed. Considering the observations, 95% of net radiation partitioned to LH and 2% of net radiation partitioned to SH, while CLM partitioned 66% of net radiation to LH and 31% of net radiation to SH.

Because there were no energy flux measurements in the dry plots during 1992–1993, we could not show the energy flux responses to water limitation. We show here the results from six-paired ambient and FACE, four-paired high N and low N to compare our model simulation to the observation. CLM generally underestimated the energy flux responses to elevated CO2 and nitrogen limitation, especially for the SH and LH fluxes. Elevated CO2 reduced observed LH by −20.1 W/m² and increased SH by 16.8 W/m², while CLM

| Table 5 | Observed and Simulated Net Radiation, Latent Heat Flux, Sensible Heat Flux, and Ground Heat Flux Averaged Across February–May |
|---------|-------------------|-------------------|-------------------|-------------------|-------------------|
| Net radiation (W/m²) | Latent heat flux (W/m²) | Sensible heat flux (W/m²) | Ground heat flux (W/m²) |
| Obs | CLM | Obs | CLM | Obs | CLM | Obs | CLM |
| 902 | 121.69 | 127.73 | 124.05 | 89.68 | −1.66 | 38.19 | −1.14 | −0.14 |
| 904 | 116.30 | 128.06 | 102.32 | 85.54 | 14.46 | 43.08 | −3.08 | −0.56 |
| 906 | 130.96 | 124.93 | 131.12 | 86.52 | −0.70 | 38.45 | 0.53 | −0.04 |
| 908 | 125.70 | 125.89 | 110.23 | 83.20 | 13.76 | 43.04 | 1.71 | −0.35 |
| 909 | 137.26 | 128.46 | 128.19 | 86.48 | 4.47 | 39.18 | 4.28 | 2.81 |
| 910 | 143.33 | 128.52 | 163.73 | 86.59 | −21.80 | 39.07 | 1.24 | 2.86 |
| 911 | 135.05 | 130.97 | 100.66 | 87.28 | 24.38 | 41.74 | 4.15 | 1.95 |
| 912 | 141.62 | 131.17 | 154.32 | 87.72 | −12.85 | 41.48 | −0.02 | 1.97 |
| 913 | 133.50 | 124.52 | 115.72 | 81.03 | 9.64 | 38.48 | 8.16 | 5.01 |
| 914 | 137.56 | 129.92 | 159.00 | 86.99 | −25.29 | 39.01 | 3.86 | 3.93 |
| 915 | 129.98 | 125.06 | 81.66 | 79.38 | 37.33 | 40.73 | 11.00 | 4.95 |
| 916 | 135.84 | 132.22 | 152.31 | 87.82 | −11.85 | 40.98 | −4.59 | 3.43 |
only showed 1.1 W/m² reduction in LH and 3.1 W/m² increase of SH due to elevated CO₂ (Figure 3a). Nitrogen limitation largely reduced LH by 50.8 W/m² and increased SH by 36.9 W/m², while CLM only showed 3.7 W/m² decrease of LH and nearly no changes of SH (Figure 3b).

4. Discussion

We calibrated CLM using one treatment and then applied the calibrated parameters to the other treatments. The simulations were largely improved by the calibrated parameters, but still the observations had large phenology variations that were not well captured by CLM. CLM was only affected by the growing degree days, which is a function of temperature. The bias in the simulated phenology indicated there are other factors besides temperature and growing degree days that affecting variations on phenology in reality. Some of the phenology variation between ambient and FACE treatments was due to the blower effects (Pinter et al., 2000) that act as a frost protection fan that increased the night time temperature through mixing the cold surface temperature with warmer air temperature and resulted a warmer nighttime temperature that accelerated the phenology in the FACE treatments. The anthesis date was 2–4 days earlier, and the physiology maturity date was 2–7 days earlier in FACE than control treatments during 1992–1994. Since 1995, the control plots were also equipped with blower fans to maintain similar boundary layer meteorology as the FACE plots, so the phenology difference between control and FACE plots was not obvious. Management treatments also affected phenology. Limiting levels of water and nitrogen accelerated anthesis and physiology maturity dates by 1–7 days.

The inability to simulate the accelerated phenology at FACE treatments resulted in an inconsistent bias in estimating the elevated CO₂ effects on grain weight. The observed increase of grain weight gradually declined during the grain fill period. Such an inconsistent response of observed grain weight was due to the phenology difference (FACE entered grain fill earlier than the ambient treatments due to blower effects). For example, on 5 April 1994, the FACE high-irr treatment showed zadocs stage 69 (completed anthesis) and grain weight 136.6 kg/ha, while the ambient high-irr treatment showed zadocs stage 62 (just entered anthesis). CLM showed a consistent increase of grain weight during the grain fill phase. Therefore, CLM underestimated the grain weight response to elevated CO₂ during the early growing season.

Many crop model validations did not focus on LAI response to elevated CO₂, because LAI simulation is not as critical for the crop growth and yield simulations. However, as a land surface model that provides the boundary conditions for atmosphere, LAI simulation in CLM is critical because of its influence on the surface energy fluxes. Our analysis suggested CLM did not simulate the factors that could reduce growth under elevated CO₂. Here, we discuss three cases that may limit the leaf growth under elevated CO₂ (Figure 4). The goal here is not to provide the possible solutions for the overestimated leaf growth response but rather to understand the uncertainties of leaf growth response to elevated CO₂. First, elevated CO₂ may affect the
sink size. CLM adopted a maximum allowable LAI (LAI_{max}) to limit leaf growth, which is equal to 7 m^2/m^2 beyond which there is no response to any environmental conditions. Whether elevated CO₂ affects LAI_{max} is unknown, but through a sensitivity test that reduced LAI_{max} to 5.5 m^2/m^2 for the FACE treatments (kept 7 m^2/m^2 for ambient treatments) to represent a sink limit, we found the LAI response to CO₂ decreased from 27.7% to 9.2%. Second, elevated CO₂ may affect leaf senescence. During 1992–1994, FACE treatments entered grain fill stage 3–4 days earlier than ambient treatments due to the previously mentioned blower effect. The blower effect was fixed by adding blower fans in the ambient treatments as well as FACE during the 1995–1997 experiments, whereby the accelerated phenology became less obvious, i.e., only 1 day earlier start of the grain fill stage. We increased the leaf senescence rate for the FACE treatments and LAI response to CO₂ reduced from 27.7% to 13.4%. Third, elevated CO₂ may affect the leaf traits, such as the SLA. Many other observations on natural vegetations reported the reduced SLA in response of elevated CO₂, although this was not the case at Maricopa FACE site. We found that reducing SLA from 0.028 to 0.018 m^2/g largely reduced LAI response to CO₂. LAI in the FACE treatments was lower than the ambient treatments. The response reduced from 27.7% to −7.2% (Figure 4).

To understand whether there is any interaction between stimulated LAI and photosynthesis, we performed additional simulations for one ambient (902) and one FACE (904) treatment with a version of CLM that can be run with prescribed LAI. We prescribed the FACE LAI to be the same as ambient LAI, while still increased CO₂ to 550 ppm (we called this simulation CLM4.5_SP). We found the stimulated LAI further promoted photosynthesis in response to elevated CO₂, but such promoted photosynthesis disappeared when the crop entered the grain fill stage. From January to March, CLM4.5 simulated 20–35% higher LAI under elevated CO₂, which resulted in 21–41% higher photosynthesis and −7.3% to 0% lower LH flux (Figure 5a). The increase of photosynthesis due to elevated CO₂ was 50% lower when LAI was not increased by elevated CO₂. LH flux showed a stronger decrease (−2 to −8%) when LAI was not changed (Figure 5b). From April to May, when the crop entered grain fill stage, CLM4.5 had the same leaf senescence rate for ambient and elevated CO₂. The previous positive feedback disappeared where stimulated photosynthesis did not contribute to increasing LAI. During the grain fill stage, the stimulated photosynthesis showed a similar increase rate in CLM4.5 as in CLM4.5_SP.

Beside the large positive response to elevated CO₂, CLM showed insufficient response to irrigation. Crop growth at low-irr treatments was not largely reduced (during 1993–1994) or even unaffected (during 1992–1993). The amount of irrigation applied in 1992–1993 was much higher than in 1993–1994. When
The FACE Wheat Project first started in 1992, a huge amount of irrigation water (317 mm) applied into both the low-irr and high-irr treatments after planting in order to germinate the seeds near the surface from the subsurface drip irrigation system (in subsequent years, a portable sprinkler irrigation system was used to provide the initial water for germination). Such high irrigation resulted in high soil moisture, which was well captured in CLM (Figure 6a). During the high soil moisture time period, the low-irr and high-irr treatments showed no big difference in above ground biomass. Later in the grain fill stage, the averaged observed soil moisture contents were 0.24 and 0.31 m$^3$/m$^3$ for low-irr and high-irr treatments, while they were 0.31 and 0.36 m$^3$/m$^3$ in the CLM simulation. Even though CLM showed the soil moisture difference between the low-irr and high-irr treatment, there was no soil water stress with such high soil moisture. During 1993–1994, the soil moisture was underestimated in December and January, which resulted in a smaller increase of soil moisture than if the early season soil moisture was well simulated. The simulated soil moisture at low-irr treatment well matched the observed from days 52 to 90, when LAI was smaller at low-irr than high-irr. During the grain fill stage, the simulated soil moisture was also quite large for the low-irr treatments during 1993–1994 (Figure 6b), so crop growth at low-irr treatments was only reduced slightly. The reason for the higher simulated soil moisture in CLM could due to model underestimating plant water uptake, which has been reported by other studies that CLM could not adequately simulate the role of vegetation control on soil moisture and LH flux (Lu & Kueppers, 2012; Williams & Torn, 2015). These previous studies showed CLM overestimated soil evaporation while underestimated plant transpiration. A dry surface layer that increased soil evaporation resistance has been implemented (Swenson & Lawrence, 2014) in a recent version of CLM, which may improve the crop growth response to irrigation.

Even though CLM could underestimate LH, the LH observations may not reflect the actual LH. The Maricopa FACE site was equipped with net radiometers and soil heat flux plates to measure net radiation and soil surface heat flux, respectively, and SH flux was calculated from the temperature difference.

**FIGURE 6.** Observed and simulated soil moisture variations during (a) 1992–1993 and (b) 1993–1994 for low-irr (orange) and high-irr (green) treatments.
between air and surface, as well as the aerodynamic resistance from wind speed as described in (Kimball et al., 1994; Kimball et al., 1995). LH flux was the residual, so it was subject to measurement errors from several instrument errors, although net radiometers and infrared thermometers were rotated weekly between the control and FACE plots to minimize some of the errors. Averaged across observations from February to May, 97.4% of available energy (net radiation minus ground heat flux; Rn-G) partitioned into LH and only 2.6% into H. Such partitioning is not typical for crop sites among FLUXNET sites, which have direct measurements of SH and LH using eddy covariance technique. For example, a winter wheat site at Oklahoma (US-ARM) showed 60.5% of available energy partitioning into LH and 39.5% partitioning into SH from February to May. However, irrigation and advected heat could have increased the LH. An irrigated corn site in Nebraska (US-Ne1) showed 73% of available energy (Rn-G) partitioning into LH and 27% partitioning into SH for the growing season during April–September. None of them are close to the high energy partitioning into LH at the Maricopa FACE site, which is surrounded by desert.

5. Conclusion

In this study, we validated the CLM spring wheat growth response to elevated CO2, irrigation, and nitrogen fertilization using data from the Maricopa spring wheat FACE experiments. CLM underestimated above ground biomass by 7% (117 g/m²) and overestimated grain yield by 13% (91 g/m²). CLM showed an overall too positive growth response to elevated CO2 but insufficient growth response to irrigation. In response to elevated CO2, the season-averaged LAI was increased by 27.7% in CLM, but observed values actually decreased by 0.6%. Grain yield was increased by 26.2% in CLM, but only 14.2% was observed. Observations showed elevated CO2 stimulated grain yield higher at limiting irrigation but reduced them at limiting nitrogen fertilization. CLM also showed such responses to elevated CO2 interactions with irrigation and nitrogen fertilization, but the magnitudes of grain yield changes were generally too strong except at low nitrogen fertilization. The insufficient response to irrigation was due to CLM underestimating LH flux during April and May, which resulted in higher soil moisture. Therefore, there was little or no water stress with low irrigation. In response to nitrogen fertilization, but overestimated grain yield increase.

We also validated the energy flux responses to elevated CO2 and nitrogen fertilization. The observations showed LH flux was reduced (−20.1 W/m²) with elevated CO2 but increased with nitrogen fertilization (50.8 W/m²). CLM agreed with the direction of such changes but with much less magnitude. Simulated LH flux was reduced by 1.1 W/m² by elevated CO2 and increased by 3.7 W/m² with ample nitrogen fertilization compared to the limiting treatment. The poor simulation of the energy fluxes was partly due to CLM underestimating vegetation controls on transpiration and partly due to the use of the residual energy balance method for determining LH flux, which likely partitioned too much energy into LH flux.

Based on these validations, we summarize a list of further model developments that are required for CLM to better simulate crop growth:

1. Add a leaf senescence process during vegetative phase.
2. Modify the stem area index calculation, where SAI is determined by stem weight.
3. Modify the carbon allocation when LAI reaches the maximum.
4. Adopt a dynamic SLA that responds to environmental changes.
5. Add a representation of chaff weight.
6. Add a stem senescence process during the grain fill phase.
7. Implement a dynamic carbon allocation that responds to elevated CO2, irrigation, and nitrogen fertilization.
8. Implement dynamic controls on phenology that respond to other environmental factors than just temperature.
9. Increase the vegetation controls on LH flux.

Some of these developments are directly related to the existing crop growth routines, but some of them will require development of new modules within CLM. Some of them can be done easily, but some of them may require more observations.
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