**Evaluating the Community Land Model in a pine stand with 13CO2 labeling and shading manipulations**

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Jiafu Mao1,\*, Daniel M. Ricciuto1, Peter E. Thornton1, Jeffrey M. Warren1, Anthony W. King1, Xiaoying Shi1, Colleen M. Iversen1 and Richard J. Norby1

[1] Evironmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

***\**** Corresponding author: (Tel: +1-865-576-7815, [maoj@ornl.gov](mailto:maoj@ornl.gov))

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**Abstract.** Carbon allocation and flow through ecosystems regulate land surface–atmosphere CO2 exchange and thus is a key, albeit uncertain, component of mechanistic models. The Partitioning in Trees and Soil (PiTS) experiment-model project tracked carbon allocation through a young *Pinus taeda* stand following pulse-labeling with 13CO2 and two levels of shading. The field component of this project provided process-oriented data that was used to evaluate and improve terrestrial biosphere model simulations of rapid shifts in carbon allocation and hydrological dynamics under varying environmental conditions. Here we tested the performance of the Community Land Model version 4 (CLM4) in capturing short-term carbon and water dynamics in relation to manipulative shading treatments, and the timing and magnitude of carbon fluxes through various compartments of the ecosystem. When calibrated with pretreatment observations, CLM4 was capable of closely simulating stand-level biomass, transpiration, leaf-level photosynthesis, and pre-labeling 13C values. Over the 3-week treatment period, CLM4 generally reproduced the impacts of shading on average soil moisture at 15-95 cm depth, transpiration, relative change in stem carbon, and soil CO2 efflux rate, although some discrepancies in the estimation of magnitudes and temporal evolutions existed. However, the calibrated version of CLM4 lacked the model structure to track the progression of the 13CO2 label from the atmosphere through foliage, phloem, roots or surface soil CO2 efflux. This model bias arises, in part, from the lack of a short-term non-structural carbohydrate storage pool and progressive timing of within-plant transport. By confronting land surface models such as CLM with intensive field manipulations, we can help to identify model strengths and weaknesses, model uncertainties, and additional observations necessary for future model development.

**1 Introduction**

Accurate projection of the changing global climate, given a particular scenario of future greenhouse gas emissions or concentrations, is largely determined by adequate representation of mechanistic processes in Earth System Models (ESMs) (Taylor et al., 2012). Land Surface Models (LSMs) and their associated biogeophysical and biogeochemical parameterizations are key determinants of the ESMs’ fidelity in characterization and quantification of the complex feedbacks in the Earth System (Arora et al., 2013; Friedlingstein et al., 2006; Pitman, 2003). Modeling groups have increasingly used observational data and mechanistic knowledge of processes to advance the development of LSMs (Best et al., 2011; Dai et al., 2003; Krinner et al., 2005; Oleson et al., 2013; Wang et al., 2011). Global and regional observations of land surface fluxes, states, and dynamic vegetation change offer insights into the large-scale interactions between the land surface and atmosphere, and hence facilitate model improvements at relevant scales in space and time (Beer et al., 2010; Huntzinger et al., 2012; Luo et al., 2012; Randerson et al., 2009). However, to better quantify and reduce uncertainties arising from deficiencies in model process representation, parameters, driver datasets and initial conditions, there has been significant effort to evaluate and to calibrate LSMs against site-scale observations and experimental manipulations (Baldocchi et al., 2001; De Kauwe et al., 2014; Hanson et al., 2004; Ostle et al., 2009; Raczka et al., 2013; Richardson et al., 2012; Schaefer et al., 2012; Schwalm et al., 2010; Stoy et al., 2013; Walker et al., 2014; Williams et al., 2009; Zaehle et al., 2014). Further, model development from these focused site-scale studies, especially in close collaboration with experimentalists, can potentially inform and prioritize new experiments and observations that are specifically designed to advance critical terrestrial ecosystems and processes (Shi et al., 2015).

The Community Land Model (CLM) is an advanced LSM with a comprehensive mechanistic parameterization of carbon (C), water, and energy budgets for diverse land types that can be applied across multiple temporal scales (Oleson et al., 2010). It is traditionally evaluated against historical observations from a wide range of sources, and these evaluations have resulted in rapid progress toward better model performance and hence upgraded model versions (Bauerle et al., 2012; Bonan et al., 2011, 2012; Koven et al., 2013; Lawrence et al., 2011; Mao et al., 2012a, 2012b, 2013; Oleson et al., 2008; Randerson et al., 2009; Riley et al., 2011; Shi et al., 2011, 2013, 2015; Thornton et al., 2007). Nevertheless, little attention has been paid to CLM’s ability to replicate short-term manipulative experiments, which provide an avenue for exploring and validating model response to sudden, large changes in environmental drivers that control physiological and ecological responses (Amthor et al., 2001; Bonan et al., 2013). Combined model-experiment projects can focus efforts on specific mechanistic processes whose representation in the model may be neither adequate nor appropriate for specific sites (Walker et al., 2014; Zaehle et al., 2014). Extending these model-experiment evaluations and ensuing model refinements to additional sites of the same and different ecosystem types improves confidence in the regional and global scale adequacy of the LSM’s mechanistic process representation and parameterization.

Photosynthetic C assimilation, the allocation of photosynthesis products into tissues with different turnover rates, and the respiration of C back into the atmosphere are important determinants of the CO2 exchange between the terrestrial biosphere and the atmosphere (Schimel et al., 2001). Biosphere-atmosphere C exchange is dynamically mediated by weather, soil conditions, vegetation community composition and phenology, and natural and anthropogenic disturbances (Cannell and Dewar, 1994; Litton et al., 2007). Mechanistic characterization of the fate of photosynthetically-fixed C, in particular the magnitude and timing of C allocation among plant compartments, is a major challenge for experimental and modeling communities (Epron et al., 2012). Various C-allocation schemes have been proposed and implemented in LSMs to capture both the dynamic changes in C allocation and response to external conditions of C allocation (De Kauwe et al., 2014). They generally employ either fixed coefficients or in some cases dynamic coefficients that are functions of time or time-varying external conditions to allocate assimilated C to different plant components (e.g., leaves and stems). These allocation schemes and coefficients are generally not well constrained by observations. More process-based understanding, better measurement techniques, and targeted experimental manipulations are needed to better constrain allocation within the model structure and the models’ overall representations of C dynamics.

Carbon isotopes provide important constraints on specific processes and can be used in labeling experiments to track pulses of carbon through plant and soil components. 13C as measured in plant pools is a useful constraint on stomatal conductance because of its effects on photosynthetic discrimination (Farquhar et al., 1989). Exposing plants to 13C enriched CO2 and provide important constraints on simulated C allocation (Ehleringer et al., 2000). The post-treatment carbon isotope composition (δ13C) of organic matter and respired CO2 acts as a tracer of plant C allocation (Atkin 2015; Bahn et al., 2012 and accompanying papers). The ability of a model to simulate observed patterns of the 13C-tracer is a measure of how well the model simulates the allocation of C fixed by photosynthesis. As indicated above, improved simulation of C allocation has consequences for better simulating ecosystem C storage and CO2 exchange with the atmosphere. When incorporated into the LSMs of ESMs, the improved simulation of ecosystem C dynamics improves the simulation of global coupled carbon-climate feedbacks with the inherent implications for modeling future climate change. Model improvement of course first requires the identification of model strengths and weaknesses.

Our specific goal was to test the representation of C uptake and short-term allocation patterns of a site-scale, point version of CLM version 4.0 (PTCLM) (Oleson et al., 2013) at an experimental field facility in Oak Ridge, Tennessee, USA. The “Partitioning in Trees and Soils” (PiTS) project exposed a young loblolly pine (*Pinus taeda*) stand to a pulse of air enriched with 13CO2, then tracked that label from the foliage through photosynthetic uptake, through the stem and roots and ultimately out of the soil as respiratory flux (Warren et al., 2012). Comprehensive ancillary data were collected both before and after the labeling treatment (Warren et al., 2013). In addition, over a three-week period, shade cloth was used in a treatment to determine the impact of solar radiation, and resultant abrupt GPP reduction, on allocation. One-half of the trees received light shading (68% of ambient photosynthetically active radiation (PAR) passed through the shade cloth), while the other half received heavy canopy shading (11% of ambient PAR passed through the cloth).

Model evaluations are complicated by the concurrence of parametric and structural uncertainty, which confounds the attribution of model errors (Keenan et al., 2011). A model’s performance might be negatively impacted by misrepresentation of mechanistic processes, poor parameterization of otherwise sound functional representations, or both. Parameter optimization, however, can help to isolate structural deficiencies in the model. In this study, we applied model calibration, by optimizing model parameters, as a tool to highlight areas for model development rather than simply improving predictive skill. We optimized selected CLM parameters against pretreatment data. We then evaluated the performance of the calibrated CLM in the pretreatment phase and again in the post-treatment phase without recalibration following simulation of the canopy shading and 13CO2 treatments. Our intention is that by applying robust parameter optimization to the pretreatment simulations we will reduce parametric uncertainty (Fox et al., 2009; Ricciuto et al., 2011), leading to greater insight regarding model structural uncertainty in evaluation of the post-treatment results.

The manuscript is organized as follows: We first describe the observational data sets, the model, and the simulation design. We then present results comparing the model results with the field observations; we continue with a discussion of model limitations revealed by the simulations and implications for potential model improvement. We conclude with recommendations on designing future manipulative field experiments to further improve model performance.

**2 Methodology**

**2.1 Experimental site description and observations**

The project was conducted in a young loblolly pine stand at the University of Tennessee Forest Resources AgResearch and Education Center in Oak Ridge, Tennessee. The soil is classified as a silty-clay-loam (13.3% sand; 35.7% clay; 51.0% silt), with bulk density ranging from 1.2 to 1.4 g cm-3 at 10 to 70 cm depth. One-year-old seedlings (1 g C m-2 (Griffin et al., 1995)) were planted at 2.5 × 3 m spacing in 2003, and the experiment was conducted in 2010 when the trees were ~7 m tall.

In 2010, a subset of eight of the trees, adjacent to one another, and their soils, were instrumented with automated sensors to continuously measure soil temperature, soil moisture vertically throughout the soil profile, soil surface 12CO2 and 13CO2 efflux, root production at 10 and 30 cm depths, stem sap flow, and stem diameter (Warren et al., 2012). Various measurements were manually collected periodically, including predawn foliar water potential, photosynthetic light- and CO2-response curves, root biomass, growth, and mortality, and soil C and nutrient content. Meteorological data were collected every 30 minutes at 2 m height in an adjacent open field, and included wind speed, air temperature, photosynthetically active and shortwave radiation, precipitation, and relative humidity. Additionally, in order to assess conditions under the shade cloth treatments (described below), short-term measurements of wind speed, temperature, and humidity were collected at the canopy surface following shade cloth installation. Linear regressions between meteorological data from under the shade cloth and from the open field were used to estimate conditions at the canopy surface during the experimental period (Fig. 1a, b). Results indicate wind speed (u) was ~45% (± 15%; ± 1 *SD*) lower, relative humidity (Hr) was ~6% (± 5%; ± 1 *SD*) greater, and temperature (T) was ~0.11°C (± 0.82 °C; ± 1 *SD*) lower under both levels of shading as compared with the adjacent open-field meteorological station.

Following several weeks of pretreatment measurements, the eight study trees were enclosed with plastic film stretched over a frame surrounding the trees, and then trees were exposed to 53 liters of 99 atom % 13CO2 label for 45 minutes. The plastic was removed and replaced with light shade (LS) or heavy shade (HS) cloth, each of which covered four trees and provided differential levels of PAR at the canopy surface for 3 weeks following the labeling (e.g., Fig. 1c). Pretreatment non-destructive measurements of soil moisture, soil temperature, soil respiration, sap flow and stem growth were made for several weeks prior to the labeling. For 3 weeks after the labelling and during the shading treatment, destructive measurements of foliage, stem phloem tissue, roots and soil were collected to assess presence of the 13C label, and linked to concurrent automated measurements of 13CO2 from the soil surface (Warren et al., 2012). Experimental results and additional details on the site and experimental design are in Warren et al. (2012) and datasets are available online (Warren et al., 2013).

**2.2 Model description**

We used CLM4 (Oleson et al., 2010), the land component of the Community Earth System Model (CESM) (Gent et al., 2011), to simulate the manipulated processes in the PiTS study. This CLM version includes fully prognostic carbon and nitrogen representations for its vegetation, litter, and soil biogeochemistry components (Oleson et al., 2010, 2013; Thornton and Rosenbloom, 2005; Thornton et al., 2007).

Carbon allocation in this version of CLM is simplistic. After maintenance respiration demands are calculated and subtracted from gross primary productivity (GPP), and after nitrogen downregulation of GPP is calculated, the remaining available carbon is allocated at each half-hourly time step following annually fixed ratios of leaf to stem and root carbon pools, and to resulting growth respiration. The allocation ratio between stem and leaf is a function of the previous year’s net primary productivity (NPP), while all other allocation ratios are fixed throughout the simulation for a given plant functional type. For 13C, photosynthetic fractionation is calculated and photosynthetically fixed 13C is immediately allocated to plant pools following the above description. There is no further fractionation in within-plant processes or during decomposition (Oleson et al., 2013).

Several major developments of CLM performed specifically for this study include: (1) introducing the ability to represent the shade effect and experimental labeling by driving the model with observed atmospheric 13CO2 concentrations, where before 13CO2 was assumed to be a constant fraction of CO2, (2) developing a site-level simulation workflow that leverages PTCLM capability to reproduce actual field experiments, (3) calibration of the selected model parameters to improve predictions and reveal structural errors, and (4) adding functional unit test capability for the photosynthesis subroutines.

**2.2.1 Description of PTCLM simulation**

To perform simulations at the PiTS site, we used PTCLM, a scripting framework to run site-level simulations of CLM efficiently with site-specific forcing and initialization data (Oleson et al., 2013). We performed the standard 600 years of accelerated decomposition spinup, in which soil organic matter decomposition rates are increased (Thornton and Rosenbloom, 2005), followed by 1000 years of normal spinup, in which the decomposition rates are returned to their normal values, and a transient simulation between 1850-2010 using historically varying CO2, 13CO2, nitrogen deposition, and aerosol forcing data. During both spinup and transient phases, we cycled 11 years of observed climate data. Long-term meteorological driver data were not available at the PiTS site, and instead were taken from the nearby Walker Branch and Chestnut Ridge eddy covariance sites (Hanson et al., 2004) for the years 2000-2010. On January 1st, 2003, we simulated a disturbance by harvesting the existing forest and manipulating the model restart file to capture planting of seedlings using a biomass of 1 g C m-2. The model then simulated the young stand through the year 2010. For the spinup and transient phases through 2002, default temperate evergreen needleleaf model parameters were used. Beginning in 2003, model parameters were modified via calibration (see below) to simulate the planted Lobolly trees.

To simulate the treatment period, we replaced the meteorology from the eddy covariance sites with observed data at the treatment sites starting at day of 13CO2 labeling in September 2010 (Warren et al., 2012). The 13CO2 pulse was applied in the model (assuming 100% 13CO2) during a time matching the labeling period. Incoming longwave radiation, which is a required CLM input, was not measured. We assumed that the heavy shade cloth emitted downward longwave radiation at a blackbody temperature similar to that of the air temperature, and that the light shade cloth did not impact incoming longwave radiation significantly. In the light shade case, we therefore applied the model’s internal estimate of incoming longwave radiation, which uses clear-sky assumptions about atmospheric temperature and emissivity (Idso, 1981). These assumptions were verified by later measurements of both the light and heavy shade cloths with an infrared camera (data not shown).

**2.2.2 Model calibration for pre- and post-treatment periods**

We first calibrated the model to simulate the pretreatment conditions using observations and prior information about model parameters. Data constraints for the calibration consisted of single pretreatment estimates for leaf, stem, and root biomass from allometric relationships for similarly aged loblolly pine (*Baldwin*, 1987; *Naidu et al.*, 1998; *Vanlear et al.*, 1986), a pretreatment δ13C measurement for leaves, a pretreatment δ13C measurement for bulk roots, and daily sap flow and soil respiration observations from each of the 20 days preceding the 13CO2 labeling and shading treatments. Because CLM predicts canopy transpiration but not sap flow, daily transpiration during the experiment was estimated by scaling the sap flow measurements using sapwood area and ground area covered by the rooting system (Wullschleger et al., 2001; Warren et al., 2011). Here we assume the rooting system of each tree occupied 7.5 m2 of ground area based on the spacing between the trees. For consistency purpose, the sap flow is hereafter called transpiration for both the observational and modeled results.

Some model parameters were estimated directly from observations (Table 1). Other parameters for which more direct estimation was not possible were optimized to maximize fit between model results and the observed calibration data (Table 1). The selection of parameters for optimization was based on formal sensitivity analysis (Sargsyan et al., 2013) and prior experience with the model. We defined the sum of squared errors (SSE) between simulation and observations weighted by data uncertainty as the cost function for the optimization. We used a genetic algorithm (Runarsson and Yao, 2000) to find a set of parameters that minimizes the cost function. Simulations were performed in parallel using 2 populations of 32 ensemble members in parallel over 100 iterations for a total of 6400 model simulations.

For the pretreatment (pre-labeling) period, we compared the standard version of the model (PRE-STD) with the optimized version (PRE-OPT). The model with optimized parameters was used in simulations for the shading treatment period for both the high shade and low shade treatments. Because of uncertainties associated with simulated stomatal conductance and transpiration in high-shade conditions, we performed additional parameter calibrations for the parameters mp (slope of the Ball-Berry stomatal conductance formulation) and bp (intercept of the Ball-Berry stomatal conductance formulation) during the shade treatment period using the genetic algorithm with transpiration and stem growth data as constraints (HS\_MB), with results discussed below.

**2.2.3 Evaluation of CLM photosynthesis functions**

There is considerable value in evaluating fundamental processes in CLM, and other models, at more than one scale or level of system organization. Evaluating the model’s representation of photosynthesis, for example, at both the leaf and whole canopy or stand level can provide insights into the model’s scaling relationships (e.g., the integration of leaf photosynthesis through the canopy). However, limitations of the current code structure make it tedious to examine the functional representation of processes in CLM at scales or levels below that of the stand/ecosystem/plant function type for which the model normally generates output. This is especially true if the evaluation requires multiple runs of the model under, for example, different environmental conditions, with alternative parameter values, or for optimization. Accordingly, Wang et al. (2014) have developed a functional unit testing platform allowing direct comparison between the output of functional processes simulated by CLM and the corresponding field observations. In brief, the functional unit testing isolates targeted CLM processes and functional units (e.g., subroutines) into standalone modules that can be run with specified environmental conditions and parameter values without executing the entire CLM framework. The platform then provides links with observational data against which the functional unit simulations can be evaluated. Further details can be found in Wang et al. (2014). Here we used the functional unit testing framework to evaluate CLM’s representation of the photosynthetic light response at the scale of the individual leaf against light-response curves obtained by Warren et al. (2012) for foliage in the upper canopy of trees at the PiTS experimental site prior to the shade treatment.

**3 Results**

Mean surface air temperature adjacent to the site decreased from Day -20 to 4 (“negative” days refer to days prior to the addition of 13CO2 and shading treatments), then recovered somewhat and remained without obvious trend but with variation for the rest of the post-labeling period (Day 5 to 25) (Fig. 2a). Peak 13CO2 concentration occurred on Day 0 as a consequence of the short-term labeling event (Fig. 2b). The impact of the shading treatments (Day 0 to 25) on shortwave radiation was noticeable (Fig. 2b).

The model predicted exponential growth in all biomass pools during the 8 years pretreatment, with perhaps some slowing in the final year (Fig. 3a). Compared to the CLM results with standard parameters, C stocks of the simulation with optimized parameters were lower and closer to observation-based estimates of leaf, stem and root biomass (Baldwin and Feduccia, 1987; Naidu et al., 1998; Vanlear et al., 1986). Before parameter optimization, the photosynthesis module of CLM overestimated observed net assimilation at the leaf level under moderate and high PAR conditions, which is consistent with the biomass being too high in that simulation. With optimization, assimilation was reduced, especially at PAR greater than approximately 250 µmol m-2 s-1 (Fig. 3b). Optimization substantially improved agreement with observations at higher PAR, albeit with some loss of agreement at light levels below approximately 200 µmol m-2 s-1 (PRE\_OPT simulations, Fig. 3b). Overall, the CLM-simulated light-response curve using the PRE\_OPT parameterization was in better agreement with the observed light-response curve. It should be noted that the improvement was realized with parameters optimized against stand-level observations (Section 2.2.2) and not the leaf-level observations of photosynthesis, which served as an independent validation of the optimized model.

Using parameters optimized against the pretreatment data, soil temperature predicted by CLM at 0-5 cm depth had a consistent overestimation bias of 1-2 °C, but the model closely reproduced the daily variation and decreasing tendency in surface soil temperature in both the pretreatment and post-treatment periods (Fig. 4a). No clear influence of shading treatments on this soil state variable was seen in either the observational data or model simulations. Substantial variability in observed soil moisture (integrated for 15-95 cm depth) was found among samples taken near different trees under the same shading treatment (Fig. 4b). Observed LS soil water was lower than that of the HS soil water at the start of the treatment period, probably because of local differences in soil properties and pretreatment evapotranspiration. The difference between observed LS and HS soil water content increased during the treatment period, suggesting reduced evapotranspiration in the HS plots, as supported by observations of slightly reduced transpiration under HS relative to that under LS (Fig. 4c). Following precipitation events on Days 7, 10, and 15, both observed and simulated soil water content increased (compare Fig. 2a, 4b). CLM systematically overestimated the magnitude of soil water content by 6-8% (units are volume % of water in soil), but it captured the reduction in LS soil water during the treatment period compared to the HS treatment. Before the implementation of shade treatments, the trees assigned to HS were observed to have higher transpiration than the LS trees (Fig. 4c), likely a consequence of the higher biomass and leaf area of the HS trees (Warren et al., 2012) and perhaps also higher soil water content (Fig. 4b). We used the pretreatment transpiration data to calibrate CLM, and the model simulated the pretreatment observations well in terms of both magnitude and temporal variations (Fig. 4c). After the treatment initiation, decreased transpiration was seen in both observations and model simulations for the HS and LS trees. For the LS case, CLM captured the observed transpiration well. However in the HS case, CLM predicted a sharp reduction in transpiration, whereas the observations differ relatively little from the LS case. To investigate this difference further, we performed a second optimization for the Ball-Berry stomatal conductance slope and intercept terms (HS\_MB). However, despite increasing these parameters to near the maximum acceptable values (Table 1), the HS\_MB optimization failed to reproduce the measured transpiration.

In contrast with the continued increase of stem carbon in the observed LS trees, the stem carbon of the observed HS trees declined over the shading treatment period (Fig. 5a). The model captured that basic difference in the observed response of stem carbon to HS and LS, but overestimated the rate of change under LS and simulated an essential halt in growth under HS rather than the observed decline in growth. The shorter-term (3-5 day) variation in stem carbon (based on diameter change) under shading (Fig. 5a) we attribute primarily to precipitation events and changing soil moisture (Fig. 2a and Fig. 4b), and the accompanying swelling and shrinkage of stem diameter, which translates through the allometric functions to apparent changes in stem biomass. The model displayed almost no short-term variability in stem carbon - the model does not represent stem swelling and shrinking with water status.

Both observed and simulated soil respiration tended to decline over the study period (after Day-10 in the observations) (Fig. 5b). We attribute that decline to corresponding decreases in temperature and soil moisture (Fig. 4a, b). The tendency for that change in environmental conditions to slow or reverse itself between Day 5 to 10 (Fig. 4a, b), appears to be reflected in a slowing or halting of the decline in soil respiration, especially in the model but also in the observations (Fig. 5b). The pretreatment soil respiration beneath the trees chosen for the HS treatment was 30% higher than under those selected for the LS treatment. After the application of the shade treatments, relative differences between the observed HS and LS soil respiration were reduced, but respiration from HS soil remained higher. In contrast, simulated soil respiration was slightly higher under LS, although the difference is quite small. The observed temporal variability in soil respiration under both HS and LS was not well simulated, especially the increase following precipitation events. Neither CLM4’s carbon allocation to roots nor its predicted root respiration is dependent on soil water conditions. CLM4’s heterotrophic contribution to soil respiration may also have too little sensitivity and the timing of soil respiration response to soil water variation may also be too simplistic.

The observed foliar δ13C increased above pretreatment background values almost immediately on Day 0 (the day of labeling), with slightly higher initial values under LS, followed by an exponential decline such that δ13C of LS and HS were similar by Day 8, and δ13C of LS was lower than the HS by day 20 (Fig. 6a). Because the shading did not take place until after the labeling, observed differences in foliar 13C are caused only by differences in leaf structure, photosynthetic rates and discrimination between the LS and HS trees. The model produced nearly equal foliar uptake of δ13C on day 0 in the LS and HS treatments. Neither the HS nor LS simulations captured the magnitude of the immediate spike and subsequent decline seen in the observations; simulated foliar δ13C increases but does not spike with the simulated enrichment remaining nearly steady throughout the treatment period. Simulated points reflect daily average values. The lower magnitude of the simulated Day 0 value compared to subsequent days, reflects the fact that labeling was initiated near midday and on Day 0 the model experienced both background and enriched 13C concentrations. The model does capture the fact that LS δ13C declines faster than the high shade δ13C. In the simulation, this occurs in the LS case because of the dilution of the δ13C pulse with new photosynthate allocated to the leaf carbon pool. In the HS case, shading sharply reduces GPP, and nearly all photosynthate is allocated to maintenance respiration rather than structural carbon pools.

The observed phloem δ13C peaked by Day 2 for both levels of shading, with greater enrichment in HS (Fig. 6b). In contrast, the model exhibited essentially no increase in phloem (live stem C in the model) δ13C under either shade treatment and little difference between LS and HS. In both simulations, phloem δ13C changed little compared to observations, through the shading period (Fig. 6b). As with leaf δ13C, phloem δ13C in the LS case declines faster than in the HS case, also likely representing a dilution effect in the simulation. However, the observations indicate an opposite effect for phloem δ13C.

There was no consistent shade treatment effect in the observed δ13C of bulk fine-root samples (Fig. 6c), although after a few days, bulk roots were enriched over background under both treatments. On Day 20, observed δ13C values in the fine-root pool were still higher than the background δ13C levels, especially in the LS treatment. The model overestimated the background bulk root δ13C for the pretreatment period by 2‰. As with foliar and phloem δ13C, after Day 1 bulk root δ13C values remained nearly stable in the HS simulation and slightly declined in the LS simulation, again representing dilution by new photosynthate.

The simulated δ13Cefflux from soil increased immediately with peak values on the labeling day (Day 0) for both treatments (Fig. 6d). These model results are inconsistent with the observed peak δ13C values occurring on Day 3 for LS and Day 4 for HS. Observed δ13C of soil CO2 efflux decreased exponentially after the peak under both treatments. The model, on the other hand, simulated decreases of δ13C soil CO2 efflux to near pretreatment levels immediately following the peak values and under both treatments returned to background levels by Day 1. A slight rising trend in both the simulated HS and LS cases represents the turnover of labeled leaf and fine root litter.

**4 Discussion**

**4.1 Pretreatment model results and implications**

The optimized model significantly improved simulations of pretreatment tree biomass and transpiration (Fig. 3a). This was as expected since we used those observations in our parameter optimization. Perhaps not so expected, calibration with these observations improved leaf-level performance. Optimized parameters (Table 1) controlling stomatal conductance changed little from default values for the temperate evergreen needle-leaf plant functional type (PFT). The pretreatment simulated leaf 13C in the optimized model is also close to the observation (Fig. 6a), providing additional validation for these stomatal conductance parameters and evidence that photosynthetic discrimination is being handled well in CLM. Simulated bulk root 13C is slightly too high (Fig. 6c), indicating possible errors in root turnover time, or the model’s failure to account for post-photosynthetic fractionation (Badeck et al., 2005). The fine-root to leaf allocation ratio increased from 1.0 to 1.24, which is well within the range of reported values (White et al., 2000). The fraction of leaf nitrogen in RuBisCO was 70% higher than the model default value, and while on the high end, is consistent with measurements of other loblolly pine trees (Tissue et al., 1995). The temperature sensitivity of maintenance respiration (Q10mr) nearly doubled from the default value of 1.5 to 2.83. This is higher than most values in the literature but is consistent with the value of 2.71 reported by Hamilton et al. (2001) for loblolly pine, although this value only pertains to leaf respiration. This higher Q10 value is also more consistent with the leaf-level photosynthesis data. The stem to leaf allocation ratio also is higher in the optimized model than in the default model. This is consistent with the fact that Loblolly trees are valuable for timber, as they are able to grow a large amount of wood for a relatively low leaf area index.

Though several changes in the canopy photosynthesis scheme were made in the version 4.5 of CLM (*Bonan et al.*, 2011; *Oleson et al.*, 2013), in this work, the canopy photosynthesis process of CLM4.0 did a reasonably good job against our evaluation metrics, including the leaf-level light response data. These data provided an important benchmark, since they were not used in the optimization (Fig. 3b). We found that the parameters most consistent with the biomass, transpiration, soil respiration and δ13C data were also consistent with these leaf-level data, which gives confidence in both the model’s ability to simulate the shading effect, and the model’s ability to scale leaf-level processes to the canopy.

**4.2 Treatment model results and implications**

Early simulations of the shading treatment (not shown) were naively forced with reduced incoming shortwave radiation without any adjustment to the longwave radiation. This resulted in vegetation temperatures that were lower than the observed air temperatures, high leaf boundary layer relative humidity, and nearly zero transpiration. This model limitation inspired additional measurements of the shade cloth with an infrared camera, showing that the cloth emitted longwave IR with a blackbody temperature near the observed air temperature. Using a modified forcing for longwave radiation (Fig. 1, 2), we produced more realistic simulations for the HS treatment. The shade cloth used for the LS treatment was found to have little impact on IR, thus the original forcing was used for this treatment.

The lack of large differences in soil moisture between the LS and HS simulations is likely due to a combination of error in model inputs and weaknesses in model structure. Specifying a single site-specific soil texture may not have captured spatial heterogeneity in soil biophysical properties, and it has been noted CLM4 process representation may have limitations in its ability to capture realistic site hydrology (Li et al., 2011). The small difference between shading treatments in the observations of soil moisture (note the scale in Fig. 4b), albeit larger than the simulated difference, may be due to a measurement artifact. It is known that there was some overlap of LS and HS roots that could dampen the differences in soil water between treatments. This was ameliorated in subsequent PiTS projects by trenching and lining the trench with plastic film to isolate the treatments. However, soil moisture did not significantly impact carbon uptake or allocation in the simulations at this relatively wet site. Moreover, the large variability in observations of soil water suggests that the small differences between treatments in mean soil water are likely not significant.

The observed decrease in transpiration with shading (Fig. 4) was affected by the shade treatment’s impact on shortwave and longwave radiation and a coincident reduction in air temperature (Fig. 2). This effect was reproduced well in CLM for the LS case. However, observations do not show a strong response of transpiration in the HS case but the model transpiration is highly reduced (Fig. 4c). Assuming that carbon assimilation is strongly reduced in the HS case as shown in the leaf-level light response curve (Fig. 3b), this implies a strong reduction in water use efficiency, which is not captured by the Ball-Berry conductance model as implemented in CLM (De Kauwe et al., 2013; Oleson et al., 2010, 2013). The HS\_MB optimization for stomatal slope and intercept parameters has little effect on transpiration despite increasing these parameter values well beyond reasonable ranges (Table 1; red line in Fig. 4c). The failure of the model under these conditions suggests a possibility that there is a diurnal or circadian control on conductance that is decoupled from photosynthesis and not currently captured. Another possibility is that there exists a strong nonlinearity in the relationship between stomatal conductance and net photosynthesis, which has been observed at low light levels and strongly impacts estimated transpiration (Barnard and Bauerle, 2013). Errors in modeled leaf temperature and leaf boundary layer vapor pressure deficit may also contribute to the discrepancy with observations, indicating a need for expanded environmental measurements in future work. Conductance may have been maintained to some extent by vapor pressure differences between the foliage and the shade cloth – indeed, dew was observed on unshaded trees in early morning, yet not on the shaded trees, indicating a differential temperature gradient that was not modeled. The behavior of stomatal conductance under low light has important implications for the carbon and energy balance, and the choice of conductance models has a strong impact on future predictions in climate models (Damour et al., 2010). More experimental results are needed to evaluate the effects of low-light conditions on stomatal conductance and the accuracy of current model representations of these effects. There may also have been pretreatment differences between the LS and HS trees that our assumptions in translating from sap flow to transpiration did not capture. Attention to pretreatment characterization in subsequent experiments with this translation might reduce this uncertainty.

The model’s carbon allocation to the stem may be less sensitive to short-term variation in environmental conditions than whatever contribution to observed (allometrically defined) variations in stem biomass as a result of actual stem growth and respiration (Fig. 5a). Stem diameter can shrink or swell based on changes in stem xylem water content, bark water content, and cambial growth, and is dependent on xylem water potential, vapor pressure deficit, C availability, non-structural carbohydrate concentrations, and C allocation (Vandegehuchte et al., 2014). C allocation to stem growth is revealed by a step-wise increase in stem diameter that occurs in response to favorable conditions, and that is maintained under less favorable conditions. The LS treatment clearly displayed the step-wise increases in stem diameter, while the HS treatment displayed a reduction in stem diameter. The shrinking stem diameter of HS trees indicates a decline in xylem and phloem water content likely linked to phloem sugar concentration. The HS treatment certainly reduced foliar C uptake and C available for phloem loading and allocation to cambial growth (Warren et al., 2012). The model bias towards too much growth, or too little decline in growth does indicate that the treatment of allocation is too simplistic in CLM. Seasonal patterns of allocation are known to occur (Epron et al., 2012), while the allocation scheme in CLM is quite simple, using annually invariant ratios to allocate available carbon to leaf, stem, fine-root and coarse-root pools. Capturing the correct patterns of allocation (both where to and from which plant compartments, and when) is crucial for accurately modeling carbon fluxes, pool sizes, and associated climate feedbacks (De Kauwe et al., 2014; Epron et al., 2012; Litton et al., 2007). It is clear from this study that additional work is needed to improve allocation routines in CLM.

CLM allocates all newly-assimilated carbon to plant pools and to growth/maintenance respiration every half-hourly model time step, while lags of several days are observed in this study. The resulting gap between modeled and observed C allocation was particularly evident in the model simulation of immediate 13C enrichment in autotrophic and heterotrophic C fluxes. Plant storage pools in the form of non-structural carbohydrates play an important role in regulating the allocation to structural pools, and may make up a significant portion of total biomass (e.g. Hoch et al., 2003). Simple models that account for non-structural carbohydrates better compare with observed 14C and stem growth, indicating the importance of the pools over seasonal to decadal timescales (Richardson et al., 2013) in addition to the short timescale of this study. It will be important in future work to implement a short-term non-structural carbohydrate storage pools and a representation of within-plant transport of these pools along with a more realistic allocation scheme to capture these lags, as well as interactions of C allocation with environmental driving conditions. Also, modeled δ13C of soil CO2 efflux was too high on the first day of labeling and too small afterwards. This high simulated efflux represents a pulse of growth and maintenance respiration from the coarse and fine root pools, which is the result of near instantaneous allocation of assimilated carbon. The efflux that was observed after the labeling may also include a contribution from root exudates, which could be a significant fraction of net primary productivity (Högberg et al., 2010) and have significant implications for carbon and nutrient cycling. Given the deficiencies of the current model, there are clear model development needs to address the model’s allocation to roots and the root’s utilization of that carbon, and a need from the experimental community to provide relevant observations across a range of biomes and timescales to test and develop global LSMs.

**4.3 Implications for experimental design**

A closer connection between carbon cycle modeling and experimental design is needed to systematically target the largest model process uncertainties systematically and also to improve predictive understanding. Modeling can inform experimental design by indicating where the largest uncertainties exist, while new data from experiments can constrain model predictions or lead to the integration of previously unconsidered processes. Considering model needs as part of the experimental design process (e.g., necessary drivers, and even the units in which variables are reported) can greatly facilitate the use and increase the benefits of experimental data. At the same time, considering the ability to simulate real-world experiments is best done as part of the model design process.

This model-experiment interaction highlighted some limitations of this first PiTS observational dataset that have already had implications for subsequent efforts. New experiments in a dogwood stand are addressing several issues based on knowledge gained from the PiTS 1. Additional observations include multiple treatments in different seasons, a collection of absolute destructive tree biomass at the end of the study (rather than estimates based on allometric relationships), seasonal leaf-level photosynthetic measurements, assessment of mycorrhizal C flux, and improved meteorological measurements. Although model parameters can be improved through optimization as in this study, ideally model parameters should be measured when possible. These additional observational data are necessary for more detailed model evaluation and improvement of model routines of C and allocation patterns at various time scales.

In addition to measuring model parameters, we also found that the initial seedling biomass was very important for simulating pretreatment biomass in this young forest in an exponential growth phase. This finding reinforces the understanding that models like CLM can be very sensitive to initial conditions, especially in systems, which are not in approximate or quasi- steady state. When designing experiments with an eye towards close engagement with models and the comparison of model and experimental results, attention should be given to measurements of the model’s initial conditions as part of the experimental pretreatment characterization.

It is also critically to evaluate global LSMs at a wide range of scales. Evaluating models against experiments that include measurements at multiple scales (e.g. leaf level and canopy level) should lead to increased confidence. Although LSMs quite reasonably focus on, and generate output for, aggregate whole-stand properties such as stand-scale net ecosystem exchange and evapotranspiration, many experimental observations are made at finer scales involving individual components of the stand or ecosystem (e.g., individual leaves). It is often difficult to evaluate models using a consistent framework across these scales. As used in this study, the functional unit testing allows for model evaluation at the empirically accessible scales of experimental field observations (Fig. 3b). Stand-level manipulation experiments targeted towards improving LSMs should not neglect including fine-scale measurements.

**5 Conclusions**

The point version of CLM4 was successfully implemented, calibrated and evaluated against carbon and hydrology observations from the PiTS experimental manipulations at the 7-year-old loblolly pine trees. Our results demonstrate the important role of CLM4 physiological parameters (e.g., those listed in Table 1), initial carbon states (e.g., seedling biomass), driver data (e.g., the incoming longwave radiation), and internal algorithms (e.g., the allocation routines) in determining the performance of water and C flux and dynamic C allocation simulation. These systematic process-based evaluations through intimate linkage between model and experiment facilitate the identification of the model limitations and uncertainties. While the model is able to capture the pretreatment biomass and leaf-level responses, its capability in reproducing the observed daily patterns of allocation revealed by the 13C labeling experiment is still limited. Model development efforts should focus on improving the timing and magnitude of allocation patterns. Furthermore, the model was not able to reproduce the observed high-shade treatment effects, which resulted in strongly reduced transpiration but only slightly reduced productivity. Finally, this short-term model-experiment synthesis helped to inform and prioritize new complementary long-term observations in a follow-on experiment, including seasonal carbon allocation and partition patterns and seasonal A/Ci curves, for future CLM evaluation, calibration and improvement.

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**\* stem-leaf allocation is a function of annual NPP. 2.2 is the nominal value at NPP = 800 gC m-2 yr-1**

**Captions of Tables and Figures**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **parameter** | **description** | **units** | **ENFT default** | **PRE\_OPT** | **HS\_MB** |
| *measured* |  |  |  |  |  |
| slatop | Top of canopy specific leaf area | m2/gC | 1.00E-02 | 1.02E-02 | 1.02E-02 |
| dsladlai | Change in SLA through per unit LAI | gC-1 | 1.25E-03 | 0 | 0 |
| leafcn | leaf C:N ratio | gC/gN | 35 | 50 | 50 |
| *optimized* |  |  |  |  |  |
| mp | Ball-Berry stomatal conductance slope | none | 6 | 5.59 | 71.3 |
| bp | Ball-Berry stomatal conductance intercept | mol m-2 s-1 | 5000 | 4960 | 61100 |
| froot\_leaf | fine root to leaf allocation ratio | none | 1 | 1.24 | 1.24 |
| stem\_leaf | stem to leaf allocation ratio | none | 2.2\* | 3.29 | 3.29 |
| flnr | fraction of leaf N in RuBisCO | none | 0.05 | 0.0845 | 0.0845 |
| q10\_mr | maintenance respiration t-sensitivity | none | 1.5 | 2.83 | 2.83 |
|  |  |  |  |  |  |

**Table 1.** Default PFT-level, site-specific and optimized parameters for the PiTS site used in CLM 4.0. PFT-level parameters are for the temperate evergreen needleleaf forest type. Optimized values were obtained using the pretreatment data (PRE\_OPT), and for the transpiration data during the shading period (HS\_MB). In the HS\_MB optimization, only the mp and bp parameters were optimized, while other parameters retain their pretreatment optimization values.

**Figure 1** (a) Air temperature (T, °C), relative humidity (Hr, %) and (b) wind speed (u, m s-1) under the shade cloth at the top of the canopy compared with open field measurements at 2 m height; (c) Typical diurnal patterns of photosynthetically active radiation (PAR, μmol m-2 s-1) at the site under full sun, light shade or heavy shade treatments.

**Figure 2** (a) Daily air temperature (°C) and precipitation (mm d-1) for the pretreatment and treatment of light shade (LS) and heavy shade (HS) (Day -20 to 25), (b) change in daily atmospheric long wave radiation (LW, W m-2), short wave radiation (SW, W m-2) and 13CO2 (PPMV) prior to and after exposure to shade treatments. Dashed gray line represents the starting day of the treatment.

**Figure 3** (a) CLM simulated change of leaf carbon (PRE\_STD\_LeafC), stem carbon (PRE\_STD\_StemC) and root carbon (PRE\_STD\_RootC) with default parameters, and change of those (PRE\_OPT\_LeafC, PRE\_OPT\_StemC and PRE\_OPT\_RootC) simulated with optimized parameters for the pretreatment period between year 2003 and Sep. 1st (dashed gray line) of year 2010. Observational estimations of leaf (OBS\_LeafC, which are 221.1 g C m-2, 283.8 g C m-2 and 181.9 g C m-2), stem (OBS\_StemC, which are 1011.2 g C m-2, 973.8 g C m-2 and 1220.1 g C m-2) and root (OBS\_RootC, which is 488.4 g C m-2) are based on measured stem diameters at breast height and allometric relationships from similarly aged loblolly pine (*Baldwin*, 1987; *Naidu et al.*, 1998; *Vanlear et al.*, 1986). Note that y-axis is log10-scaled. (b) Comparison of observed and simulated light response of top of the canopy leaves of loblolly pine at the PiTS-1 site. Solid black circles are mean ± 1 std dev of observations. Solid red and green circles are simulated results from the net photosynthesis module of the functional unit testing framework using site-observed parameters (PRE\_STD) and optimized parameters (PRE\_OPT), respectively (see section 2.2.2). Simulations are with the mean observed internal CO2 concentrations (Ci) and leaf temperatures (Tleaf) at the observed light (PAR) levels and the site’s observed leaf nitrogen (Na).

**Figure 4** (a) Observed (obs) and CLM simulated (sim) daily soil temperature at 0-5cm depth (standard deviation, *SD* = 0.6-1.4 °C), (b) volumetric soil water content at 15-95cm depth (±*SD*) and (c) the transpiration before and after initiation of light shade (LS) or heavy shade (HS) treatments (*SD* = 0.1-1.7 mm day-1). “HS – opt” represents the CLM simulation with optimized leaf conductance parameters. The vertical dashed lines indicate the starting day of the shade treatments.

**Figure 5** (a) Observed (obs) and CLM simulated (sim) daily stem carbon relative to day 0 (±*SD*), and (b) soil respiration prior to and after exposure to light shade (LS) and heavy shade (HS) treatments (±*SD*). Both observed and simulated stem carbon were normalized to 1 at Day 0. The simulated soil respiration is the combination of autotrophic respiration from roots and heterotrophic respiration from the decay of litter and soil organic matter. The vertical dashed lines indicate the starting day of the treatments.

**Figure 6** (a) Observed (black) and CLM simulated (blue) change in δ13C (parts per thousand (‰)) of (a) leaf, (b) phloem, (c) bulk root and (d) soil surface efflux δ13C for the light shade (LS, open circle) and heavy shade (HS, filled circle) pretreatment and treatment periods (± standard error (SE)). The modeled δ13C values were calculated from the CLM simulated 13C and 12C variables and the reference standard (0.0112372) using the equation described in https://en.wikipedia.org/wiki/Δ13C. The 13CO2 labeling pulse was initiated on Sep. 1st in year 2010 (Day 0). Dashed gray line represents the starting day (again Day 0) of the shading treatment. To better visualize the model results, inset figures illustrate the CLM simulated δ13C values for the light shade (open triangle) and heavy shade (filled triangle) treatments from Day 1 to Day 25.