Response Letter

Dear Editor and reviewers,
Thank you for your constructive comments and suggested changes for improving our manuscript. We do appreciate your thoughts and insights and believe the result is a significantly improved manuscript.

Reviewer #1 (Comments to Author):
In this paper, the authors attempt to reproduce observations of canopy behavior during a shading experiment following introduction of a pulse of high-concentration $^{13}CO_2$ and subsequent shading treatments. The results are that CLM performs better in pretreatment conditions when tuned to site-specific values, and CLM is unable to capture the observed track of the $^{13}CO_2$ pulse through the canopy and roots. The finding that tuning improves model performance at a site is hardly new or novel. This has been done many times before (e.g. Collello et al., 1998; Prihodko et al., 2008; Rosolem et al., 2012, and many more).

Response: As emphasized in those references the reviewer listed, we agree that improving the model parameters is one of the most important and effective ways for model development. But as you can see, our effort on optimizing CLM parameters for the pre-treatment period is not the only story for this study. We found that even with the updated model parameters there were still some differences between the simulated and observed variables especially during the treatment period. So, by isolating the impact of model parameters, we addressed that those errors should be mainly attributed to structural model uncertainties, which can illuminate further model developments. We have modified the text to better explain the purpose of parameter optimization (Section 2.2.2).

The following of ^{13}C through the system is the more interesting component of the paper, and, in my opinion, a lost opportunity. Instead of describing what the observations mean with respect to the behavior of the natural canopy, the authors simply gave a clinical description of how the model differed from the observations. “We ran a model, here’s what happened.” Come on. I can think of a conceptual model whereby the ^{13}C pulse is first taken up by the leaves, then takes time to work through the system. You can see some of this in Figure 6, particularly 6(a) and 6(d), but the behavior in the phloem and bulk roots is more subtle and complex. But a description of processes and mechanisms at work in the real canopy are never addressed, and the reason for model departure from observations is glossed over, the authors merely saying that the allocation scheme “needs attention” and a more labile storage pool should be added. Isn’t this the time to do it? I would be very interested to see a paper that demonstrates the mismatch between modeled and observed ^{13}C, posits some reasons for the mis-match, addresses them, and runs the model again. That would be a very interesting paper.

Response: We understand the point, and we wish we could do all the model evaluation, development and calibration in one paper. However, we think this manuscript adds value to the community by introducing the capability to perform a detailed model-experiment comparison using a global land-surface model. This study adds new capability to CLM in particular: (1) the explicit use of the $^{13}CO_2$ observational information by reading new stream file rather than assuming fraction of CO_2 as in the default CLM version, (2) improvement of the site-level simulation structure and leverage of the capability for single-point implementation of the Point Version of CLM (PTCLM), (3) calibration of the selected model parameters for the pretreatment period with parameterization optimization techniques, and (4) accomplishment of the functional test capability for the photosynthesis subroutines and multi-scale evaluation using both leaf and canopy scale data. But as you can see from the title and content of this paper, we have mainly focused on the evaluations (not just the carbon isotopes but other important carbon and hydrological variables) of the CLM model with the unique PiTS manipulations for the first phase of our CLM-PiTS work. To achieve this purpose, we have conducted a lot of novel work that is unique in the land-surface modeling community, and worth reporting as a separate paper. We have improved the Results and Discussion parts to place our paper more in the context of relevant canopy processes. A successful LSM model development effort will require that we understand these processes across broad temporal and spatial scales. A forthcoming manuscript will use not only the short-term datasets of this PiTS 1 experiment but the subsequent PiTS 3 experiment. Both experiments (and other published work) will be used to develop and test a new C partitioning regime in CLM – one that allows short-term C storage pools that can reflect abrupt shifts in GPP, seasonal changes in ratios of C allocation to different pools, and inclusion of additional C sinks such as fruit or fungal symbionts. So, in the updated version, we further developed a conceptual model for photosynthate transport based on the experimental observations, and discussed conditions under which the hypothesized mechanisms could have an important influence on model behavior in larger-scale applications.

No real discussion was given for why we are interested in simulating carbon isotopes through the ecosystem. Is it simply to gain a better understanding of biogeophysical processes? Could we expect to see better simulation of net carbon flux and/or the Bowen ratio with better understanding of ^{13}C? Are there implications for ecosystem response to changing climate?

Response: Our interest in accurately simulating carbon isotopes through the ecosystem is not simply, or even primarily, to gain better understanding of biogeochemical processes. Rather we are interested in using the isotope tracer to identify areas of improvement specifically in the model representation of carbon allocation, and thus to improve the representation of C storage and CO_2 exchange with the atmosphere, with the implications for simulation of climate-carbon feedbacks and future climate when these improvements are incorporated into ESMs. We have added text in the Introduction (lines 118-125) outlining this interest, the why, of our interest in simulating carbon isotopes in the ecosystem.

My initial inclination is to recommend rejection for this paper, but I think there is an opportunity here. Take out, or at least minimize the sections on parameter tuning. The community has already done this. A more detailed focus on what is going on with the isotopes as they move through the real system is needed, as is discussion of model success/failure in reproducing the observations and what it means. Finally, the authors should hypothesize some ways to modify CLM, and implement them. This would result in some actual hypothesis testing, as opposed to a paper that reads “We ran a model: here’s what happened.” My formal recommendation is acceptance with major revisions.

Response: As suggested, we reduced the parameter optimization related part and placed it in the context of the ultimate goal of evaluating the model structure. We also added some sentences on the importance of isotope study, and presented potential model developments that could reduce the uncertainties and biases of the CLM in isotope simulations.

Specific Comments:

The unit testing was mentioned as being very important, but not described. If the Wang (2014) paper is all the reader needs to know, cite it and move on. If more detailed description is needed, share it with the reader.

Response: A more detailed description of the functional unit testing approach for photosynthesis has been added (Section 2.2.3).

Increasing the Ball-Berry slope and intercept parameters to extreme values made little or no difference in the one plot where they were shown (Figure 4c). Obviously, then, this was not the reason for model error. Why not just say that modifying the BB parameters made no difference and move on? Also, after demonstrating that the BB parameters were NOT important, the authors state in the conclusions that they ARE. This is a contradiction.

Response: The mp and bp parameters were shown to be very important for the pretreatment optimization against the observed transpiration, but that optimization did not solve the low transpiration bias for the strong shade plots in the treatment period. Lines 522-563 of Section 4.2 were added to discuss the possible reasons behind the failure of the Ball-Berry approximation during the treatment period.

Wording in the Conclusions was modified to better reflect the main point of this result.

Figure 6: there is no explanation given for del 13C, the y-axis on all plots. The scale amplitude differs by an order of magnitude between the panels; the reader needs to be told what is going on here. I'm assuming that the standard treatment is used, where the sample 13C/12C ratio is compared to a standard; is it PDB? Not all readers are isotopists, so some description and context would be helpful. The change of the del value from negative to positive might confuse some readers, so more explanation is warranted.

Response: We added a brief description of the calculation of del ^{13}C in the caption of Figure 6.

Where did the carbon isotope treatment come from? I'm familiar with Suits et al. (2005) and van der Veld et al. (2014). Does the CLM methodology follow these or something else?

Response: The treatment most closely follows Suits et al. (2005). A complete description is provided in Section 25 of the CLM 4.5 Technical Note (Oleson et al., 2013).

The del of the respiration is extremely dependent on the spinup, and changing del ^{13}C through the industrial era. How was this treated?

Response: The Suess effect is modeled using changing global atmospheric ^{13}C and ^{12}C from 1850-present as input. Model spinup was performed using pre-industrial ^{13}C values and default model parameters for soil carbon turnover. The text has been modified to clarify the simulation procedure (Section 2.2.1).

In section 4.2 the authors say ". . .modeled soil CO_2 efflux was too high on the first day of labeling and too small afterwards." Actually, Figure 5b shows this to be false. In actuality, the del 13C was too high on the first day, and too small afterwards (Figure 6d).

Response: Changed as suggested.

References:

Oleson, K., Lawrence, D. M., Bonan, G. B., Drewniak, B., Huang, M., Koven, C. D., Levis, S., Li, F., Riley, W. J., Subin, Z. M., Swenson, S., Thornton, P. E., Bozbiyik, A., Fisher R.,. Heald, C. L, Kluzek, E., Lamarque, J. -F., Lawrence, P. J., Leung, L. R., Lipscomb, W., Muszala, S. P., Ricciuto, D. M., Sacks, W. J., Sun, Y., Tang, J., and Yang, Z. -L.: Technical description of version 4.5 of the Community Land Model

(CLM), NCAR Technical Note NCAR/TN-503+STR, The National Center for Atmospheric Research (NCAR): Boulder, CO, USA,420 pp., 2013.

Suits, N. S., A. S. Denning, J. A. Berry, C. J. Still, J. Kaduk, J. B. Miller, and I. T. Baker: Simulation of carbon isotope discrimination of the terrestrial biosphere, Global Biogeochem. Cycles, 19, GB1017, doi:10.1029/2003GB002141, 2005.

Reviewer #2 (Comments to Author):
General Comments:

This paper combines a site level manipulation experiment (PiTs) of a young loblolly pine plot in Oak Ridge, Tennessee as a tool to test the model structure of CLM4. The authors use observations from two levels of shading to evaluate ecosystem response, and inject highly enriched $^{13}CO_2$ into the atmosphere to evaluate model allocation of carbon biomass. The authors find that through calibration of a subset of parameters that the biomass pools, respiration and transpiration are captured fairly well. Based upon differences between del13C concentration in biomass pools and del13C in the soil respiration the authors determine that the existing fixed annual allocation methodology within CLM is insufficient to represent the observed patterns in carbon allocation. They recommend the inclusion of a non-structural carbohydrate pool to help delay the allocation of carbon to plant tissue. In addition they recommend a dynamic allocation sub-model that is influenced by environmental conditions rather than the existing fixed annual allocation approach.

Response: Thanks for the nice understanding of our work described in the paper.

This reviewer felt it was unclear how the model was initialized from the spinup-phase to the sapling state in 2003. Was a disturbance imposed and/or the biomass characteristics of the sapling simply prescribed into the model? In addition, it was also left unclear which sets and how much of observed data were used in the calibration phase and which were withheld (e.g. the light response data). Although the authors demonstrate that the existing formulation is deficient in simulating allocation timing, it was less clear whether this formulation was insufficient in simulating multi-year to decadal allocation. I would have welcomed more discussion of model skill in terms of the model simulation of biomass variables from 2003-2010 against observations (Figure 3) to help contribute to this discussion. The data is already there in Figure 3, it just needs to be evaluated, and perhaps shown more clearly than in a log plot.

Response: Detailed answers can be found below in the responses to your specific comments.

Finally, C13 labeling, as demonstrated here, is used as a means to an end in order to evaluate simulated allocation and timing. To that effect, C_{13}, isotopes and isotopic fractionation are not the focus of the paper, however, the author gives the impression that the model itself is a passive placeholder for C13. In reality, the model is imposing its own mechanistic representation of C13/C12 photosynthetic fractionation upon the canopy air and is actively partitioning against the heavier C13 isotope during the photosynthetic process. The degree of fractionation is dependent upon stomatal conductance, assimilation rate and nitrogen limitation, which in turn are dependent upon environmental variables. Although this fractionation mechanism may be relatively minor as compared to the overwhelming signal of the injection of enriched $^{13}CO_2$, this reviewer would have benefitted from a more careful discussion of the simulated behavior in biomass pool del13C behavior in Figure 6. How much did the modeled fractionation processes contribute to the model-data mismatch both in terms of bias and trend, if at all?

Response: This is a good point. In our significantly modified version, please find the Sections 3.3 and 4.2 for related changes corresponding to this concern.

In general, this paper represents a valuable fusion between manipulated site level experiment to test and improve CLM skill, and recommends acceptance with revisions based upon the suggestions mentioned above.

Response: Thank the reviewer for the detailed and positive comments on our work. More detailed responses can be found below.

Specific Comments:

How was the model initalized after the spinup? Was a harvest or planting initiated at 2003 or were the sapling biomass variables prescribed into the model? Only in the results section does it become clear that the simulation was started from near bare ground in 2003 and then run forward. This should be described more carefully in the methods.

Response: All aboveground biomass was removed on Jan. 1 of 2003 to simulate a harvest, and a planting occurred in 2003 using a prescribed biomass. We added a clearer description of initialization in Section 2.2.1.

Although there were many measurements taken at the site, it was unclear what were actually used for the calibration, how many data points, and at what temporal resolution.

Response: The variables used for pretreatment calibration are described in the Section 2.2.2. We also added the temporal information associated with these observational variables in the newly added Table 2.

Page 6979, Line 19: Should read $^{13}CO_2$.

Response: Changed as suggested.

Page 6981 Line 26: I would say standard 'parameter' CLM version, instead of just standard CLM because this is confusing whether you mean parameter or structure.

Response: This sentence together with the related paragraph was totally changed (lines 288-289 in Section 2.2.2).

Page 6985: Lines 3-6: An increase in soil respiration suggests increase in root respiration? How do you not know it isn't increased soil carbon respiration?

Response: We were mainly addressing the little sensitivity of CLM simulated root and soil carbon respiration to the soil water condition. No magnitude comparison of these two respiration were involved. In the new version, we added more discussion on the soil respiration related differences (lines 575-595).

Page 6986: lines 5-10, the fact that the model overestimates the del13C could be a function of allocation turnover time or the fractionation process itself. Did you demonstrate what the pre-treatment fractionation process is. . .? Could have taken pretreatment del13C leaf samples and gotten a baseline for the fractionation process itself. It could be useful to account for the influence of fractionation on model output, and help distinguish issues with the fractionation vs. pool turnover and allocation.

Response: The pre-treatment del ^{13}C measurements were used for model calibration. Parameters controlling both stomatal conductance and allocation were included. The leaf del ^{13}C was modeled quite well (Figure 6a). The model may display a bias in bulk root del ^{13}C (Figure 6c) because of errors in allocation timing or a failure to represent post-photosynthetic fractionation. As you can see from the new version, we put a lot of analysis (Section 3.3) and discussion (Section 4.2) on the Figure 6.

Page 6987 Line 11 The leaf level light response data was not used in calibration, but I am not completely clear what was included.

Response: For clarification of the calibration variables, please see the response above. We also add more analysis on the light response related comparison (Section 2.2.3 and paragraph 2 of Section 3.2).

Page 6987 Line 17 You found that the seedling biomass was important for the simulation, so did you use that as a calibration tool? You only show in table 1, the parameters that were being optimized, but if state variables are also optimized this needs to be included in table 1.

Response: A typical seedling biomass (1 g C m^{-2}) was used to initialize the model for each simulation, including those used for calibration. These were fixed values rather than variable parameters. While uncertainty in the initial state may be important in determining calibrated parameters, we did not have suitable information and so used the fixed values. Section 2.2.1 was modified to better describe the initialization process.

Page 6989, line 23: "The simulation does not show any difference in respiration between LS and HS plots prior to the shading". But that's the same for all variables, shown in Figures 4,5 and 6. Why would it not be this way? Aren't these simulated exactly the same way between plots, or did you calibrate individually? It was my impression that the only thing that would make a simulation difference would be imposing different meteorological conditions at the point of shading. Nothing was different before this between the state of the LS and HS plots as far as the model was concerned. This is not the model's fault, and you would have to optimize or initialize the model based on subplot characteristics to get different pre-treatment simulations.

Response: This is correct. HS and LS plots are identical in the pre-treatment simulations and were not calibrated separately. In the actual experiment, the HS trees had slightly higher biomass and leaf area, leading to differences between HS and LS in pretreatment observations. We did not have quantitative information about the biomass components of each plot to conduct separate calibrations for HS and LS separately. Soil carbon may also vary among the plots but was not measured. We felt that this section added little to the discussion and removed it.

Page 6990 Lines 12-25: "It is clear from this study that additional work is needed to improve allocations schemes in CLM." I would tend to agree with this statement if we are concerned with diurnal scale variation (as show in this paper, and even then it doesn't seems quite so much an allocation problem, but a timing, or staging problem, i.e. assimilated carbon is too quickly allocated to biomass and respired), perhaps seasonal allocation variation (not specifically addressed in this paper). Has this been demonstrated for decadal time scale allocation and growth? Isn't a better indicator of model skill how well the biomass variables were estimated from start (2003) to treatment (2010) (Figure 3a). The log scale makes it hard to see, but it would appear that the calibrated simulation provides biomass variables consistent with observations, and isn't this the time scale more relevant for climate, perhaps the simple allocation scheme isn't bad for longer time frame..?

Response: Good point. However, we do not have annual observations of the biomass components from 2003-2010. We only know these trees grew up from one-year-old seedlings (1 g C m^{-2}) planted in 2003, and the estimated leaf, stem and roots carbon in 2010 based on the loblolly pine trees that have similar age

(Fig. 3a). Because the PiTS 1 experiment only lasted for several weeks, strictly speaking, what we've seen here for CLM errors in the timing and magnitude of C allocation should be mainly limited to the daily scale or short term. The Conclusions part was slightly changed to clarify this. We would expect to get more insights on the CLM capability in biomass simulation at longer time scale by doing detailed evaluations of the simulated biomass components again latest gridded or multisite observations (Thurner et al., 2014; Liu et al., 2015). Investigations with these datasets are actually underway, and details of which will be reported elsewhere.

Page 6992, Line 15. . ...'[the model]' is not able to reproduce the observed patterns of allocation as revealed by the ^{13}C labeling experiment." I thought this was too strong a statement: certainly the labeling experiment demonstrated deficiencies in model timing of the allocation, but ultimately this statement is based upon the growth patterns based upon DBH in Figure 5, which in itself was a proxy for biomass based on allometric assumptions and highly variable based on water status. It does seem like the model overestimates stem growth on this short time scale, but again is this consistent with longer term allocation as shown in Figure 3a? This might make for an interesting comparison if this short time scale overestimation in growth translates to 7 year allocation. The stem biomass seems to be captured quite well.

Response: Please refer to the above response for this comment. We have changed the expression of that sentence. In addition, in the new Discussion we used observations from the experiment to develop a conceptual model (hypothesis) of short-term photosynthate storage and transport, and suggested further studies that could be carried out to evaluate the generality of the hypothesized mechanisms (Section 4.2).

Figure 1: Labeling of relative humidity should be consistent. Hr and RH should be same thing. Choose one.

Response: Changed to Hr as suggested.

Figure 3a: Log scale, although convenient in order to apply all biomass simulations on one plot, makes it very difficult to assess the simulated vs. observed biomass variables. Do they agree within error. . ..hard to say.

Response: Based on this suggestion, we modified the Figure 3a, rewrote the first paragraph of Section 3.2, and added the observed biomass values in the caption of Figure 3a.

References:

Liu, Y. Y., van Dijk, A. I., de Jeu, R. A., Canadell, J. G., McCabe, M. F., Evans, J. P., & Wang, G. (2015). Recent reversal in loss of global terrestrial biomass. Nature Climate Change.

Thurner, M., Beer, C., Santoro, M., Carvalhais, N., Wutzler, T., Schepaschenko, D., Shvidenko, A., Kompter, E., Ahrens, B., Levick, S. R. and Schmullius, C. (2014), Carbon stock and density of northern boreal and temperate forests. Global Ecology and Biogeography, 23: 297–310. doi: 10.1111/geb.12125

Reviewer #3 (Comments to Author):
General comments

Mao and co-authors present an interesting study evaluating photosynthesis and C allocation parameters in CLM4.0 with data from a $^{13}CO_2$ labeling experiment in a young Loblolly Pine plantation.

Response: Thank the reviewer for the positive response to our work.

Although their efforts to evaluate process representation based on short-term experiments are novel and interesting, I'm surprised there's less introspection on the implications of their findings. It's not surprising that adjusting parameter values produces better results but as the author's stress CLM is a global model used for climate change projections. As such what are the implications of tuning up model parameters for Loblolly Pine trees?

Response: We are faced with the problem of improving global-scale models, but the vast majority of experimental and observation data, like PiTS, is at the ecosystem scale or smaller. In order to understand the structural limitations of a model like CLM, we need to simulate the experimental site to the best ability of the model at hand, which means using site-specific parameters and environmental conditions. Our efforts on optimizing CLM parameters for the pre-treatment period were made to demonstrate even with the best possible model parameters fit to this site-level pretreatment data, there were still some differences between the simulated and observed variables especially during the treatment period. This is illustrated more clearly by Table 2, which has been added. So, by reducing the impact of model parameters on model error, we emphasized that those remaining errors should be mainly attributed to structural model uncertainties, which can be used to guide future model developments. We have modified the text to better explain the purpose of parameter optimization in this context (Section 2.2.2). The process-level and parameter sensitivity understandings of the CLM model at this site are helpful to CLM development at broader spatial scales, particularly over the regions having similar climate and vegetation. The purpose of this study is to highlight deficiencies in model structure that may be relevant at large spatial scales. Future efforts will evaluate new model developments over multiple sites, such as in FLUXNET, or regionally. Though in this study we do not have the opportunity to investigate the global impacts of these parameter changes on terrestrial carbon, hydrology and energy dynamics by conducting offline or online CLM simulations, we intend to explore these topics in future work.

Should the Ball-Berry parameters in CLM be changed for all plant functional types based on these findings?

Response: This study highlights the limitations of the Ball-Berry model under high-shade conditions (De Kauwe et al., 2013; Oleson et al., 2010, 2013). This may have important implications for transpiration, and further experiments should be conducted to determine that behavior. For pre-treatment and low-shade conditions, the optimized Ball-Berry slope and intercept terms for the temperate needleleaf evergreen differ only slightly from the default (< 10%). Other PFTs would need to be investigated independently with detailed observations.

Would the modified parameters fit within observations constraints of data in databases like TRY or Glopnet?

Response: In the Discussion, we point out several references that show the optimized parameters are reasonable. For example, we cited White et al. (2000) to confirm our optimized fine root:leaf allocation ratio.

Are there larger structural uncertainties or biases in CLM that this study exposes? If so, how can they be corrected? As presented this work illustrates how models can be tuned with data, but misses a potential opportunity to draw broader conclusions or gain much insight.

Response: As mentioned above, with the parameters' impacts on model errors separated by performing the pretreatment optimization, we were able to identify the structural model uncertainties especially during the treatment period. We hypothesize that the main structural problems are 1) the failure of the Ball-Berry model to capture observed transpiration in high-shade conditions, and 2) the failure of the allocation module to adequately represent the timing and magnitude of the ^{13}C label in plant components. In the new Discussion we used observations from the experiment to develop a conceptual model (hypothesis) of short-term photosynthate storage and transport, and suggested further studies that could be carried out to evaluate the generality of the hypothesized mechanisms (Section 4.2).

Like any good study, this paper raises more questions than it provides answers, but the answers provided here are not very compelling. The authors very clearly state their objective and focus at the end of section 2.2. This is a paper that more narrowly focuses on building tools and capabilities in PTCLM to facilitate model-data comparisons from experimental manipulations and site-level observations. This is an important, valuable contribution. The aim here isn't necessarily to evaluate and improve CLM, but to build and document valuable tools that facilitate site-level comparisons. Perhaps one path forward would be to more narrowly cast the paper?

Response: Thank you for appreciating the importance of building these tools and capabilities to represent experimental manipulations in a land-surface model. While this is an important part of the manuscript, we feel that model evaluation and providing discussion of the model-data differences is an important scientific contribution. We note that the end of section 2.2 does not provide the overall objectives of the manuscript, but rather specifically our changes for CLM. We have now stated the overall objectives explicitly at the end of the Introduction. On the other hand, we feel that using the results of this single study to change the underlying structure of a global land-surface model would be premature. A synthesis of experiments and observations is needed, and potential model developments and future experiments are addressed in the Discussion.

As presented the paper seems to communicate that the authors were able to tune some parameters that modestly improved growth and photosynthesis parameterization for a particular tree species (Fig. 3), but neglected the heavy lifting of improving HUGE biases in soil physical & hydrology, plant C allocation, and photosynthesis/stomatal conductance (Figs 4-6). The authors adequately highlight these shortcomings and suggest solutions, although it doesn't really appear they're interested in addressing them in the future. One reading of this paper would conclude that by applying a novel (but incomplete) experimental design allows for fine tuning of parameters for a particular plant species that aren't really that bad in the global parameterization of CLM and highlights some huge biases and structural issues with a model that the authors can't address, or aren't really interested in fixing.

Response: We agree that an increased emphasis on implications is needed, and our revised manuscript includes several passages that highlight intended future work to address the model deficiencies and biases that were identified but not solved in our study. Other parts of this comment are more problematic. We do not agree that the parameter optimization produced only "modest" improvements in predicted growth – please note the logarithmic y-axis scale in Figure 3a, which is a typical way to show biomass accumulation curves, but which might give the mistaken impression that the reduction of bias in the optimized model was small. We also do not agree that the improvements in photosynthesis are "modest": although there is a remaining high bias around PAR=500 umol/m2/s, the biases at higher PAR are greatly reduced, and now fall within the observational uncertainty. Regarding the model performance in the area of soil physics (Fig 4): There is a consistent overestimation of soil temperature by about 1.5 °C, but the model captures the variance in soil temperature well. Prediction of soil water content is biased high by 6-8%, but the model reflects the observed variance due to wetting and drying reasonably well. The point of the paper, of course, is not to evaluate the soil physics submodel – panels a and b are included in Figure 4 to show that there are not obvious patterns in the soil physics observations or predictions that explain the difficulty experienced in simulating transpiration under the high-shade treatment. As panel 4c shows, the model does a remarkably good job with predictions of the pre-treatment and low-shade transpiration, compared to observations, but is unable to capture the high transpiration observed for the high shade treatment. This is a major finding for the study, and we have further highlighted the importance of this result in the revised manuscript. As far as we know, this type of evaluation has not been performed before, and it seems to us quite an interesting result that the model, using a very standard parameterization of canopy physics and biochemistry, is unable to capture the observed transpiration under high shade. Regarding model predictions of plant C allocation: we do not agree that the results shown in Figure 5 a represent a "huge" bias – instead our interpretation is that the general pattern of a widening spread between low-shade and high-shade treatments as the experiment progresses is captured quite well by the model. The model predictions of soil respiration (Figure 5 b) also seem quite reasonable to us, given the (typical) large uncertainties in the observations. Certainly the results in Figure 6 do show a huge bias in the dynamics of labeled carbon, and this is one of the major issues dealt with in the paper. We have added new text in the Discussion (lines 596-665) that provides a more detailed discussion of what would be needed to capture these dynamics in the model, and what could be gained by having that increased realism in the allocation module.

Specific comments

Why shading? What does this kind of manipulation tell you about model response to disturbance or environmental change? The $^{13}CO_2$ seems novel and valuable but the value of shading seems less clear, especially w/o a control during the experimental period of focus unless it's to illustrate biases in low light (nighttime?) stomatal conductance.

Response: The shading treatment was designed to abruptly reduce GPP, which will affect the internal plant C flux and C partitioning to various sinks. It was used to create a strong disturbance in observable C partitioning, which could then be used to explore model sensitivity. Measured parameters such as stem C and sap flux displayed large shifts over the three-week treatment.

It's confusing understand what features of different version of CLM were used in this study. For example, CLM4.5 (Oleson et al. 2013) documents the ^{13}C features and PT-CLM configuration used here? However, the photosynthesis, C allocation, and hydrology came from CLM4.0? It seems ironic that the authors would note the significant efforts to improve the CLM (P 6974 L 1-6), yet used a version of the model that does not reflect those changes (CLM4.0) in particular changes to canopy photosynthesis (Bonan et al. 2011, 2012) and known issues with soil hydrology in the models (e.g., Swenson & Lawrence 2014). Can this be somewhat clarified for readers not familiar with different versions and configurations of the model?

Response: CLM 4.0 was used for this study. Oleson et al. (2013) is referenced solely for the PTCLM configuration, which does not affect the model structure. Modifications of soil scheme in Swenson & Lawrence 2014 were mainly focused on the improvement of CLM over semiarid regions. Although we noted biases in the soil hydrology, there is little influence on carbon fluxes and allocation patterns since this site is not water-limited. The canopy photosynthesis in CLM4.0 does a reasonably good job against our evaluation metrics, including leaf-level light response data, and the CLM4.5 will be evaluated in future manuscripts. As suggested, some further discussion and clarification on model version were added.

The experimental design that this study is trying to replicate seems surprising to me. As I understand it there are measurements for pre-treatment, two shading experiments, and post-treatment, but during the shading experiment there's no untreated control group?! Repeating the experiment is well outside the scope of this manuscript, but a more compelling study would have been to parameterize the model for the pretreatment period and then see if it can even replicate control conditions during and after the experimental shading. This is especially troubling since the $^{13}CO_2$ pulse came at the start of the shading experiment, and for which there are no control (i.e. unshaded) data?

Response: We considered using a shade treatment and an un-shaded control treatment, but were worried about the potential differences in environmental conditions caused by the shade cloth, independent of changes in light (i.e., relative humidity, wind). Thus we decided to use a heavy shade as the treatment, and the light shade as the control. We wanted to make sure all trees received the same initial CO_2 signal, thus we applied the label immediately prior to shading, then could use the two shade levels to impact the partitioning of that $^{13}CO_2$ label. We have since performed a new study, with isolated individual trees, using shaded or un-shaded controls as suggested by the reviewer, but also included comprehensive measurements of differences in environmental conditions between each tree (leaf and air T, relative humidity, above and below the canopy, and estimates of long-wave radiation based on sky or shade cloth temperatures. Both experiments (and other published work) will be used to develop and test a new C partitioning regime in CLM – one that allows short term C storage pools that can reflect abrupt shifts in GPP, seasonal changes in ratios of C allocation to different pools, and inclusion of additional C sinks such as fruit or fungal symbionts. Our revised manuscript has an expanded description of the experimental protocol that should help to address these questions (Sections 2.1 and 2.2.2).

P 6980 L 10, I appreciate the honesty about the approach, but why was this approach chosen, instead of one that provides estimates of parameter uncertainty?

Response: This is a computational limitation, other methods that estimate parametric uncertainty (e.g. MCMC) would require a larger number of simulations and are harder to parallelize. Uncertainty quantification is an active area of research in land surface modeling. Because parametric uncertainty is not a focus of this study, this sentence was removed.

I appreciate the work that went into optimizing parameters for a young loblolly pine stand, but it's hard to see and never discussed how far off the standard configuration of the model was from observations (Fig. 3a)? Are there error estimates on the observations? If so, can they be displayed (or are they already)?

Response: We modified the Figure 3a and added the observed biomass values in the caption of Figure 3a. Also, in the first paragraph of Section 3.2, we rewrote the biomass related comparison.

I understand the focus of this paper is on biogeochemistry and C fluxes but how well does PTCLM handle water and energy fluxes? How do changes in parameter values influence transpiration rates, latent and sensible heat fluxes? Has anyone looked at data from 'nearby Walker Branch and Chestnut Ridge eddy covariance sites', or other flux towers in loblolly pine plantations? At the very least there should be some introspection on how the suggested parameter changes influence other parts of the model, not just C fluxes.

Response: In addition to the C fluxes, we also evaluated the CLM simulated soil water content and transpiration against the PiTS observations. Although nearby, the Walker Branch and Chestnut Ridge sites are different vegetation types and ages, and it wouldn't be appropriate to include them in this evaluation.

Looking at soil respiration (Fig. 5) seems like a spurious analysis given the data presented. In models like this rates of respiration are largely determined by soil C pool size but as these data are never presented, it's hard to assess if the model is producing plausible results (as implied) with realistic initial states? Moreover trying to justify potential experimental differences in soil respiration seems speculative and distracts from the focus of this paper (photosynthesis and plant C allocation).

Response: Here we focus mainly on short-term variations in soil respiration, which are impacted by environmental conditions as well as the initial states. Although we don't have enough information to judge model performance in simulating soil C pools, the short-term variability is clearly not being simulated correctly. We think this is relevant in that this could be reflecting structural limitations in the model including those related to root allocation and respiration.

The authors seem to have begun this study acknowledging the C allocation scheme is and isotopic fractionation in CLM is very simple (section 2.2). Thus, findings that it does poorly against observations hardly seem noteworthy. Even still, I'm surprised the authors don't go deeper in their discussion of these results (P 6990 L 15-27). Section 4.3 reads it was taken from the DOE-MODEX website and/or a proposal the authors just submitted. No one is arguing about the value of bringing models and experiments closer together, however, this section is completely void of specific modeling needs that the results here highlight. It seems like the authors learned they need to collect some data more effectively, but it's not clear how the results from PiTS-1 inform the model development directions (and measurements) that should be prioritized. This seems like an excellent opportunity to reflect on specific knowledge gained from both model and experimental work and how that insight will be applied moving forward.

Response: As suggested and you can see, we significantly modified the Discussion part to make our point clearer.

Technical Corrections

The sentence on P 6980 L 6-7 seems incomplete. A genetic algorithm that does what? ["To reduce this possibility, we used a genetic algorithm (Runarsson and Yao, 2000)"]. Please provide a bit of background for readers not familiar with this approach.

Response: We edited this sentence for clarity.

P 6982 L 12-21. I don't completely follow this discussion. Did the authors change how CLM estimates limitations on carboxylation rates? If so, where is this described? If not, this text seems out of placed and either should be moved to the discussion or removed (with preference for the later).

Response: As suggested, we deleted several sentences beginning and after "The persistently….", and deleted the references associated with these sentences.

P 6986 L 23 Can statistics be provided for the statement that parameterized results are better than the standard configuration? This statement seems true, but the standard results don't look that bad (for using a generic evergreen pft parameterization to simulate growth of young loblolly pine stand).

Response: From our modified Figure 3a, the evident improvements with the optimized parameters can be seen clearly.

Also in section 4.1 it seems like another important parameter change is the fraction of NPP that builds stems in the optimized parameterization. This also makes sense since loblolly packs on a large amount of wood for a relatively low LAI, making it a valuable timber / plantation tree. This is never discussed.

Response: Thanks for pointing this out. We have added some text to the discussion.

Figures are small, complicated, and hard to read. In my experience this gets even worse when papers are formatted to journal styles. Can text in figures be made larger, and cluttering information (e.g. formula be put into the caption). Some of the color choices for lines are either nauseating or unreadable (green and cyan), and insets in Fig. 6 are too tiny to be useful. Please take care to generate illustrative figures that help communicate & clarify the story being told here. Where possible figures should communicate observational uncertainty. It's shown on Fig 4b, but not elsewhere.

Response: As the reviewer suggested, we have made significant changes of most figures in the updated version.

In Fig. 6, why do simulated ^{13}C concentrations seem to spike before the labeling experiment actually happened (day 0?). This an error in how the figure is drawn, how the label was applied in the simulations, or a misunderstanding on my part?

Response: The labelling happened at midday on day 0. Because CLM allocates carbon to structural carbon pools and autotrophic respiration on every half-hour time step, the spike results primarily from root growth respiration during and immediately following the labeling on day 0.

Throughout there seem to be formatting errors with the subscripts on $^{13}CO_2$.

Response: Changed as suggested.

References:

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Oleson, K., Lawrence, D. M., Bonan, G. B., Drewniak, B., Huang, M., Koven, C. D., Levis, S., Li, F., Riley, W. J., Subin, Z. M., Swenson, S., Thornton, P. E., Bozbiyik, A., Fisher R.,. Heald, C. L, Kluzek, E., Lamarque, J. -F., Lawrence, P. J., Leung, L. R., Lipscomb, W., Muszala, S. P., Ricciuto, D. M., Sacks, W. J., Sun, Y., Tang, J., and Yang, Z. -L.: Technical description of version 4.5 of the Community Land Model (CLM), NCAR Technical Note NCAR/TN-503+STR, The National Center for Atmospheric Research (NCAR): Boulder, CO, USA,420 pp., 2013.

Oleson, K. W., Lawrence, D. M., Gordon, B., Flanner, M. G., Kluzek, E., Lawrence, P., J., Levis, S., Swenson, S. C., Thornton, P. E., Dai, A., Decker, M., Dickinson, R., Feddema, J., Heald, C. L., Hoffman, F., Lamarque, J. –F., Mahowald, N., Niu, G. –Y., Qian, T., Randerson, J., Running, S., Sakaguchi, K., Slater, A., Stoeckli, R., Wang, A, Yang, Z. –L., Zeng, X. D., and Zeng, X. B.: Technical description of version 4.0 of the Community Land Model (CLM), NCAR Technical Note NCAR/TN 478+STR; The National Center for Atmospheric Research (NCAR): Boulder, CO, USA, 257 pp., 2010.

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Evaluating the Community Land Model in a pine stand with shading manipulations and $^{13}CO_2$ labeling

[Revised manuscript for Biogeosciences]

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Abstract. Carbon allocation and flow through ecosystems regulates land surface–atmosphere CO_2 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 $^{13}CO_2$ and two levels of shading. The field component of this project provided process-oriented data that was used to evaluate 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 ^{13}C values. Over the 3-week treatment period, CLM4 generally reproduced the impacts of shading on soil moisture changes, relative change in stem carbon, and soil CO_2 efflux rate. Transpiration under moderate shading was also simulated well by the model, but even with optimization we were not able to simulate the high levels of transpiration observed in the heavy shading treatment, suggesting that the Ball-Berry conductance model is inadequate for these conditions. The calibrated version of CLM4 gave reasonable estimates of label concentration in phloem and in soil surface CO_2 after three weeks of shade treatment, but lacks mechanisms needed to track the labeling pulse through plant tissues on shorter time-scales. We developed a conceptual model for photosynthate transport based on the experimental observations, and discussed conditions under which the hypothesized mechanisms could have an important influence on model

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behavior in larger-scale applications. Implications for future experimental studies are described, some of which are already being implemented in follow-on studies.

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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 characterizing and quantifying complex feedbacks in the Earth System (Arora et al., 2013; Friedlingstein et al., 2006; Pitman, 2003). Modeling studies 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;

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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 inform and prioritize new experiments and observations that are specifically designed to advance understanding of critical terrestrial ecosystems and processes (Shi et al., 2015).

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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). CLM has been evaluated against observations from a wide range of sources, and these evaluations have resulted in improved model performance (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). Processes operating over short time scales can have long-lived ecosystem consequences through indirect effects; e.g., stomatal conductance varies on timescales of hours or shorter, but indirect effects on site-level water balance through controls on transpiration can extend to annual timescales and beyond. 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

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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 photosynthetic products into tissues with different turnover rates, and the respiration of C back into the atmosphere areimportant determinants of CO_2 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, stems, and roots). 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' 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.

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Both diffusion through stomata and enzyme activity during photosynthesis discriminate against the accumulation of ^{13}C in plant tissue, making ^{13}C measurement a useful constraint on stomatal conductance (Farquhar et al., 1989). Exposing plants to ^{13}C enriched CO$_2$ can provide important constraints on simulated C allocation (Ehleringer et al., 2000). The post-treatment carbon isotope composition (δ^{13}C) of organic matter and respired CO$_2$ can serve as a tracer of plant C allocation (Atkin 2015; Bahn et al., 2012).

We evaluated the integrated response of a simulated tree-soil system to an imposed alteration of shortwave radiation, the main environmental driver for photosynthesis, and compared the observed trajectory of labeled carbon pulses through that system with approximations of carbon allocation that are typical of a global-scale model. We used a version of CLM4.0 that has been modified to allow convenient application of the global-scale modeling algorithms at single points (PTCLM, described in Oleson et al., 2013). We evaluated the model against observations and experimental results from the "Partitioning in Trees and Soils" (PiTS) experiment established in a young loblolly pine stand in Oak Ridge, Tennessee, USA (Warren et al., 2013). The project exposed a young loblolly pine (*Pinus taeda*) stand to a pulse of air enriched with ^{13}CO$_2$, then tracked that label from photosynthetic uptake, through the leaves, stem, and roots and ultimately out of the soil as respiratory flux photosynthetically active radiation (PAR) (Warren et al., 2012). We addressed two questions: (i) Is the model able to represent the biophysical and ecophysiological behavior of the experimental system in terms of pretreatment dynamics and stand-level response to the manipulated radiation environment? (ii) Do the biases inherent in a very simple model of storage and allocation propagate beyond the time scale of fast turnover storage pools? We hypothesized that it

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Deleted: (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 to reduce incident solar radiation for some of the trees; one-half of the trees received moderate shading (68% of ambient

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would be possible to parameterize the global model using site-level ecophysiological measurements, and have it realistically capture the site-level influence of the shade manipulation. We further hypothesized that, in spite of missing mechanisms to track short-term storage and allocation of C, the parameterized model could capture both pretreatment ^{13}C discrimination as well as post-treatment effects once the labeling pulse had traveled through the plant.

2 Methodology

2.1 Site description, experimental manipulation, and observations

The field component of 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 silt-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 $^{12}CO_2$ and $^{13}CO_2$ 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 CO_2-response curves, root biomass, growth, and mortality, and soil C and nutrient content. Meteorological data were

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Moved down [1]: 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.

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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.

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 % $^{13}CO_2$ 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. The LS and HS cloths were designed to allow passage of 70% and 10%, respectively, of the incident PAR.

To assess actual conditions under the shade cloth treatments, short-term measurements of temperature, humidity, wind speed, and PAR 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. Temperature was ~0.11°C (± 0.82 °C; ± 1 *SD*) lower, relative humidity (H_r) was ~6% (± 5%; ± 1 *SD*) higher, and wind speed (u) was ~45% (± 15%; ± 1 *SD*) lower, under both levels of shading than in the adjacent open field (Fig. 1a, b). The shade cloths performed very close to design, with 68% and 11% passage of PAR through the LS and HS cloths, respectively (Fig. 1c).

Non-destructive measurements of soil moisture, soil temperature, soil respiration, sap flow and stem growth were made prior to the labeling and for the duration of the shade treatment. During the shade treatment, destructive measurements of foliage, stem

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phloem tissue, roots and soil were collected to assess presence of the ^{13}C label, and linked to concurrent automated measurements of $^{13}CO_2$ 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 pretreatment and 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 et al., 2007; Thornton and Rosenbloom, 2005).

Carbon allocation in this version of CLM is simplistic. After maintenance respiration demands are calculated and subtracted from gross primary productivity (GPP), and following a step that downregulates GPP on the basis of static allocation parameters, fixed tissue C:N stoichiometry, and plant mineral N uptake, the available carbon is allocated to new growth, storage for growth in subsequent growing seasons, and associated growth respiration. The model includes pools for leaf, fine root, and several categories of stem and coarse root, with over-season storage pools associated with each of these "displayed" growth pools. The allocation ratio between stem and leaf is a function of the previous year's net primary productivity (NPP; higher fractional allocation to stem with higher annual NPP), while all other allocation ratios are fixed throughout the simulation for a given vegetation type. For ^{13}C, stomatal diffusion and photosynthetic fractionation are calculated and photosynthetically fixed ^{13}C is

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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 $^{13}CO_2$ concentrations, where before $^{13}CO_2$ was assumed to be a constant fraction of CO_2, (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 a stand-alone testing 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 CO_2, $^{13}CO_2$, nitrogen deposition, and aerosol forcing 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. These input data were cycled continuously to drive the model through the spinup and transient simulations. On model date 1 January 2003, we simulated a harvest disturbance by removing existing

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vegetation biomass and simulating planting of seedlings using a biomass of 1 g C m^{-2}. The model then simulated growth of 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 to simulate the planted loblolly trees, based on ecophysiological measurements and model calibration (see Section 2.2.2).

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 $^{13}CO_2$ labeling in September 2010 (Warren et al., 2012). The $^{13}CO_2$ pulse was applied in the model (assuming 100% $^{13}CO_2$) during a time matching the labeling period. Thermal infrared camera measurements under both light and heavy shade cloth made during various sky conditions indicated the need to modify the model input for incoming longwave radiation under the heavy shade treatment, by assuming that the heavy shade cloth emitted downward longwave at a blackbody temperature equal to the open field air temperature (data not shown). For the light shade case, we applied the model's internal estimate of incoming longwave radiation, which uses clear-sky assumptions about atmospheric temperature and emissivity (Idso, 1981).

2.2.2 Model calibration for pre- and post-treatment periods

Model evaluations are complicated by the co-occurrence 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.

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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 $^{13}CO_2$ 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.

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 $\delta^{13}C$ measurement for leaves, a pretreatment $\delta^{13}C$ measurement for bulk roots, and daily sap flow and soil respiration observations from each of the 20 days preceding the $^{13}CO_2$ 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 m^2 of ground area based on the spacing between the trees. For consistency, sap flow is hereafter called transpiration for both the observational and modeled results.

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Some model parameters were specified directly from observations (Table 1). Other parameters for which 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 ‘parameter’ version of the model (PRE-STD) with the optimized ‘parameter’ 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

Since we are interested in understanding the fate of photosynthetically fixed carbon as it is allocated to various tissues and fluxes, and how allocation dynamics respond to

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changes in photosynthesis as driven by changes in PAR, it is useful to evaluate model predictions of photosynthesis over a range of light levels. We used a functional unit testing framework (Wang et al. 2014) to evaluate CLM's representation of the photosynthetic light response at the scale of individual leaves 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. This approach isolates the targeted model process to allow a direct comparison between instrumental data and simulation output, driving the model component with specified environmental conditions and parameter values.

3 Results

3.1 Environmental forcing conditions

Mean surface air temperature adjacent to the site decreased from days -20 to 4 (day numbering is negative prior to the addition of $^{13}CO_2$ and shading treatments), then recovered somewhat and remained without obvious trend for the rest of the post-labeling period (days 5 to 25). Multiple rainfall events were recorded in the pre-treatment and treatment periods (Fig. 2a). The shortwave and longwave radiation drivers for our simulations, based on a combination of observations and estimation as described above, showed variance associated with weather patterns during the experiment, with the superimposed influence of the light and heavy shading treatments (Fig. 2b). $^{13}CO_2$

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concentrations followed historical background values except during the labeling period on day 0 (Fig. 2b).

3.2 Pretreatment and treatment evaluation

The model predicted approximately exponential growth in all biomass pools during the 8 years of pretreatment simulation, with some evidence of slowing growth in the final years (Fig. 3a). Using default global-scale ecophysiological parameters the model significantly overestimated biomass accumulation in leaf, stem, and root pools, by 85%, 36%, and 76%, respectively on Sep. 1st of year 2010 (PRE_STD curves, Fig. 3a). Replacing default parameters with observed (lower) leaf N concentration and with calibrated (higher) allocation ratios for stem:leaf and root:leaf (complete set of parameter changes shown in Table 2) brought the biomass accumulation curves in better agreement with observations (Fig. 3a). Using the PRE_OPT parameters, the bias for leaf, stem, and root biomass accumulations was -9%, -4%, and -16%, respectively, compared to observed values.

Comparison of predicted vs. observed photosynthesis light response curves was used as an independent assessment of the model performance before and after calibration across a range of PAR values characteristic of mid-day values in the open field and under the LS and HS treatments (Fig. 3b). In the range of PAR from 750 to 1588 µmol m^{-2} s^{-1}, typical of mid-day conditions in the pre-treatment period (days -25 to -1), default parameterization (PRE_STD) resulted in overestimates of photosynthesis, while data-constrained and calibrated parameterization (PRE_OPT) eliminated the bias, placing predictions within +/- 1 SD of observed values. For light conditions characteristic of mid-day values in the LS treatment (648 +/- 232 µmol m^{-2} s^{-1}) the overprediction bias for the optimized model was reduced, but at least at PAR = 500 µmol m^{-2} s^{-1} the optimized

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model predicted photosynthesis was still biased high. For the range of PAR characteristic of the HS treatment (131 +/- 47 µmol m^{-2} s^{-1}) the model with optimized parameters underestimated photosynthesis, while the model with default parameters was in good agreement (low end of the range) or was biased high (high end of the HS range).

Soil temperature predicted by the optimized model 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 near-surface soil temperature in both the pretreatment and post-treatment periods (Fig. 4a). No clear influence of shading treatments on soil temperature was seen in either the observations 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). Pretreatment observations of soil water content were not made, but observed LS soil water was lower than that of the HS soil water at the start of the treatment period, perhaps reflecting local differences in soil properties and pretreatment evapotranspiration. Although modeled soil water content at the start of the treatment was higher than observed (by 5-7%, measured as volume % of water in soil), the maximum observed and simulated excursions in soil water content between rain events during the treatment period were similar (4% and 3.5%, respectively). Predicted soil water content declined more slowly than observed during days 16-25. There is some evidence of both observed and predicted LS water content declining more rapidly than HS in this same period, suggesting higher rates of evaporation for LS than HS.

Observed transpiration during the pretreatment period was higher for HS than LS plots, likely a consequence of the higher biomass and leaf area of the HS trees (Warren et

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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 differed 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.

Both HS and LS trees showed increasing trend in stem carbon during the pretreatment period, as inferred from stem thickness measurements. While the LS stems continued to grow during the treatment period, the observed HS stem size declined (Fig. 5a). Modeled relative increase in stem carbon was more rapid during the pretreatment period than observed, and while the modeled LS trees continued to accumulate carbon during the treatment period (at a somewhat reduced rate) the modeled HS tree growth essentially stopped. The observed shorter-term (3-5 day) variation in stem carbon (based on diameter change) under shading (Fig. 5a) was attributed 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. Apart from whole-plant mortality and fire, the model has no physiological mechanisms allowing for negative growth of stems.

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Both observed and simulated soil respiration tended to decline over the study period (after Day -10 in the observations) (Fig. 5b). The observed 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 short-term variability in soil respiration under both HS and LS was not well simulated. While observations showed a reduced soil respiration coinciding with large precipitation events around Days -10, +10, and +15, simulated soil respiration rose on those days.

3.3 ^{13}C evaluation

Observations of foliar δ^{13}C show that LS and HS leaves acquired a similar concentration of labeled C, as intended by the experimental design (Fig. 6a). Observed appearance of the labeled C in phloem shows that photosynthate was rapidly moved out of leaves and into phloem, with peak observed phloem concentrations on day 2 for both LS and HS trees (Fig. 6b). Labeled C was observed in CO_2 at the soil surface, with peak concentrations around day 4 indicating a transfer through phloem to roots and metabolism belowground either as root respiration or as heterotrophic respiration of root exudate or root tissue (Fig. 6d). Increase in labeled C was observed in root tissue for both LS and HS trees, with large variability in measurements (Fig. 6c). Leaf, phloem, and root tissues showed remaining labeled C at day 20, and the label was still evident in soil surface CO_2 at day 15. For both phloem and soil surface CO_2, the LS plots showed lower label concentrations than the HS plots throughout the observed rise and fall of the labeled

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pulse. Differences between label dynamics for LS and HS roots are difficult to assess due to variability in measurements.

The model reproduced observed pretreatment values for foliar, phloem, and root tissue δ^{13}C, and for δ^{13}C in soil CO_2 flux to within 1.5‰ (Fig. 6), indicating reasonable model parameterizations for ^{13}C discrimination through the stomatal conductance and photosynthesis pathways. The model allocation approach deploys new photosynthate immediately throughout the plant to meet current maintenance and growth respiration demands. The belowground component of the modeled autotrophic respiration is seen as a large spike in labeled C in soil surface CO_2 on day 0. Other similar spikes were simulated in association with respiration of aboveground plant parts (results not shown). Lacking a representation for multi-day transport of photosynthate to sites of growth, either acropetally towards new canopy growth or basipetally towards stem or root growth, the model allocates labeled C to new growth pools immediately, where it is considered well-mixed with the existing plant tissues. There was thus a rapid increase and then a relative stabilization of the δ^{13}C label in foliage and root tissue. The model does include storage pools, which hold photosynthate for deployment as new growth in following growing seasons. Those pools were lumped for comparison to the phloem observations (Fig. 6b), and they followed a pattern similar to the predicted leaf and root tissue pools.

The model predicted a steady dilution of labeled C in leaf, root, and storage pools for the LS trees, compared to their HS counterparts. With a severe reduction in PAR, GPP was greatly reduced in the modeled HS treatment, and what little photosynthate produced was prioritized for maintenance respiration, so the label appeared quickly in tissues and remained relatively constant for that treatment. For the LS treatment GPP remained relatively high following the labeling and initiation of the shade treatment. In this case unlabeled C continued to accumulate as new growth, causing a steady decline in the label concentration for LS trees over the course of the experimental period (Fig. 6a,b,c, insets). In contrast to the plant pools, modeled soil surface CO_2 shows a gradual increase in label concentration after the initial root respiration pulse on day 0, with HS consistently showing a higher concentration of label than LS for the simulated soil surface CO_2 through the end of the treatment period (Fig. 6d, inset). The modeled process of leaf and fine root litterfall is continuous throughout the year for evergreen vegetation, and this modeled rise in soil surface CO_2 concentration of labeled C is due to litterfall and subsequent metabolism by heterotrophs.

Toward the end of the experimental period, the observed multi-day pulses of labeled C in phloem and soil surface CO_2 approached the relatively stable values predicted by the model. The observed trajectory for label concentration in leaves fell below modeled values for the final ten days of treatment. Variation in observed root label concentration toward the end of the experiment makes it difficult to assess correspondence with model results for that tissue.

4 Discussion

4.1 Assessment of model performance in pretreatment period

Default model physiological parameters most appropriate to our site are based on averages taken across numerous datasets collected in evergreen needleleaf forests. There is considerable variation within that broad type classification for all of the measured

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parameters (White et al. 2000), and any time a site-level evaluation is used to assess model behavior (as here) it is helpful to constrain within this range according to the local species or species mixture. We used measurements taken directly from the site where available, and constrained the optimization of other parameters based on the observed ranges for loblolly pine, when available. 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 (Q_{10mr}) 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. The optimized value for stem to leaf allocation ratio also is higher than in the default model, but it falls well within the observed range for loblolly pine (White et al. 2000).

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The optimized model delivered very reasonable simulations of pretreatment tree biomass, transpiration, and leaf δ^{13}C (Figs. 3a, 4c, and 6a). Including multiple independent observational metrics in the optimization cost function is a more challenging test of correct model structure, compared to optimization targeting a single model output variable (Sacks et al. 2006; Richardson et al., 2010; Ricciuto et al., 2011). The fact that our optimized model delivers good results for all three components simultaneously (biomass, transpiration, and leaf δ^{13}C) supports the notion that stand-scale model structure is reasonable.

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Independent evaluation of model results at the leaf-scale demonstrated that the optimized parameters either reduced biases (LS and open-field light levels) or gave mixed results (HS light levels) at this scale. This provides additional confirmation that the optimization approach was reasonable, and was not generating unrealistic parameter values to compensate for gross structural deficiencies in the model. This is further confirmed by the fact that optimized parameters (Table 1) controlling stomatal conductance changed only modestly from default values.

Independent evaluation of model against pretreatment $\delta^{13}C$ in phloem and in soil surface CO_2 shows good agreement, consistent with the targeted pretreatment value for $\delta^{13}C$ in leaves. Simulated bulk root $\delta^{13}C$ is biased slightly 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).

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. The ability of our optimized model to reproduce pretreatment biomass, transpiration, ^{13}C discrimination, and leaf-scale photosynthetic response to light gives confidence in the model's ability to simulate the shading effect, and the model's ability to scale leaf-level processes to growth at the whole-tree scale.

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4.2 Assessment of model performance in treatment period

We did not attempt to optimize model predictions for soil temperature or soil moisture content. The model overestimation of soil temperature while faithfully reproducing the multi-day excursions in temperature is consistent through the pretreatment and treatment periods. Soil surface temperatures were not measured, so it is not clear if the overestimation bias is related to a surface energy balance bias, to a bias in the overlying air temperature, or to parameterization error in thermal diffusivity and its relationship to soil texture and surface layer properties.

The overestimation bias in modeled soil moisture during the treatment period (there were no pretreatment observations) suggests a parameterization error for soil texture or variation in texture with depth. Small differences in the clay fraction, for example, could cause the observed offset in mean soil water content, and clearly there is variability in soil moisture states across the site, both within and between the shade treatments (Fig. 4b). We used a single estimate of sand, silt, and clay fractions from the site, and were satisfied that the model was able to capture pretreatment transpiration with that soil parameterization, and that the multi-day excursions of soil moisture were of similar magnitude in the model compared to observations during the treatment period. We also note that modeled stomatal conductance was not impacted by lack of soil water in these simulations. Periodic rainfall kept soils relatively wet throughout the pre-treatment and treatment periods, minimizing effects of bias in soil moisture on simulated photosynthesis or transpiration.

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The very large difference between modeled and measured transpiration for the HS treatment is the most confounding result from our study. All evidence indicates that the model carbon and water dynamics are well-behaved for the pretreatment period, and the model also captures the influence of light shading on transpiration accurately. Stem growth results indicate that reduced growth of LS trees, and the cessation of growth for

HS trees, is captured properly by the model. Through the Ball-Berry approximation linking stomatal conductance to photosynthetic rate, the model is forced into a state of reduced transpiration for the HS treatment, even with additional optimization that placed Ball-Berry parameters at their outer observational limits. It is possible that the sapflow measurements in the HS treatment are biased, and that the actual tree-scale transpiration is not as high as suggested by these measurements, but if true we would expect that bias to occur for both pretreatment and treatment periods, and not only to appear in the treatment period, as observed. Connected to that hypothesis, it is possible that actual leaf stomatal conductance shut down during the HS treatment, but that water continued to accumulate in the stem, moving past the sapflow sensors and filling a capacitance in the xylem tissue. However, the sustained sapflow over the long duration of the treatment period and the negative observed trend in stem diameter for HS trees argue against that interpretation.

Alternatively, if we assume that the sapflow measurements reflect actual high levels of transpiration in the HS trees, then we are forced to conclude that the Ball-Berry relationship as implemented in CLM (De Kauwe et al., 2013; Oleson et al., 2010, 2013). breaks down under these rather extreme experimental conditions. Under that hypothesis, it would seem that there is some "memory" of the expected range of light levels in the tree, and that even when photosynthesis is nearly extinguished due to experimentally forced reduction in PAR, stomatal conductance remains at a relatively high level. Another possibility is that these trees exhibit 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

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Bauerle, 2013). This type nocturnal transpiration may indeed have been greater for the HS trees if the vapor pressure deficit was larger (Domec et al. 2012). Errors in modeled leaf temperature and leaf boundary layer vapor pressure deficit may also contribute to the discrepancy with observations. 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. This hypothesis could be tested in future studies with additional leaf-level measurements under HS treatments, sampling both the diurnal cycle and the multi-day behavior of leaf physiology in trees subjected to high levels of shading. While the HS conditions are unlikely to be realized for extended periods under natural conditions, understanding this failure of the commonly-used Ball-Berry parameterization may be helpful in understanding and predicting the broader case of adaptation of stomatal behavior to environmental change, which is known to influence water and carbon cycle predictions under future climates (Damour et al., 2010).

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Deleted: , 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.

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

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certainly reduced foliar C uptake and C available for phloem loading and allocation to cambial growth (Warren et al., 2012).

The modeled difference between LS and HS in biomass accumulation in stems is in good agreement with observations based on stem diameter, with increases of 1.9% and 1.6% by treatment day 19 for model and observations, respectively (Fig. 5a). Given the previously discussed pretreatment results for biomass accumulation and leaf-scale photosynthesis, we are confident in the optimized model's ability to capture carbon dynamics at the plant scale on time scales of years to tens of days. It is reassuring to see that the model prediction of soil respiration falls in the observed range, although this could be the result of good luck as much as good performance. While soil respiration on an annual basis is closely related to litter inputs and belowground plant respiration, it is possible for compensating errors between decomposition rates and litter inputs, or between litter inputs and root respiration, to result in good model-observation agreement for the approximately monthly timescale examined here. We note a potential bias in the model relationship between soil respiration and soil moisture: while the observed soil respiration is depressed after large precipitation events, the model estimates an increase. 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. A more mechanistic treatment of water-air-microbe interactions at the scale of soil pore space might help to eliminate these differences. Resolved vertical transport of respired CO_2 in the soil column might also help to correct this bias.

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Beyond noting the obvious discrepancy in observed vs. modeled $\delta^{13}C$ dynamics associated with the lack of short-term photosynthate storage pools in CLM, we are interested in using this study to develop hypotheses explaining the observed patterns in $\delta^{13}C$, identifying the simplest mechanisms that explain observed patterns, and understanding the consequences of ignoring those mechanisms in a model like CLM. To the extent that simple mechanisms can be identified, and significant consequences of ignoring those mechanisms articulated, we leave it to future efforts to deploy and evaluate those mechanisms in new model versions and with new observational and experimental constraints.

Given that LS and HS leaves seem to have photosynthesized the pre-shading labeled pulse of CO_2 at similar rates (Fig. 6a) as intended by the experimental design, we can make some inferences about the dynamics of photosynthate storage and transport based on the timing of the pulse as it exits the foliage and passes through the phloem of the trunk, and based on differences in timing and concentration of the labeled pulse in LS and HS trees. First, the fact that observed peak label concentration is higher in phloem than in foliage, even though that peak comes two days later in phloem than in foliage, indicates that the phloem pool in the vicinity of the labeling source (the leaf) is smaller than the leaf pool itself. That is, even though the label is passing into the leaf prior to entering the phloem, the label pulse is relatively small compared to the leaf carbon pool as a whole, while it is relatively large compared to the part of the phloem pool nearest the leaf at the time of labeling. Second, the observation that $\delta^{13}C$ in foliage declines rapidly over the first ten days, and declines at about the same rate for LS and HS leaves, indicates that the movement of newly-fixed photosynthate from leaves and into phloem does not depend strongly on production of new photosynthate in subsequent days. Third, the similar timing between LS and HS trees for peak label concentration in phloem, and later in soil surface CO_2, indicates that the velocity of material movement through the phloem does not depend strongly on current photosynthesis rate. Since the HS treatment clearly reduced growth and transport belowground (Fig. 5), the logical conclusion is that the cross-sectional area of active phloem tissue responsible for transport of photosynthate away from leaves and out to roots is lower in the HS than in the LS treatment. One possible interpretation is that the rate of flow within a given phloem pathway is relatively constant, and that more phloem pathways towards the roots are active when production of photosynthate is high. A logical consequence of that arrangement would be that at any given point along the transport pathway towards the roots, or at any point in time at a given location along the pathway, the concentration of a common-sized label would be lower for a tree with high rate of ongoing photosynthesis than for a tree with low rate of ongoing photosynthesis, due to dilution of the fixed-size label into a larger number (larger cross-sectional area) of transport pathways, all with a common transport velocity (conceptual model shown in Fig. 7). This is in fact the observed relationship of LS to HS concentration at all points in time for both the phloem measurements (fixed point on the trunk) and for the soil surface CO_2, lending support to the hypothesized mechanism.

Plant storage pools in the form of non-structural carbohydrates are known to play an important role in regulating 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 ^{14}C and stem growth, indicating the importance of the pools over seasonal to decadal timescales (Richardson et al., 2013). The question remains: What are the consequences for a CLM like model of ignoring the shorter timescale (monthly) storage dynamics? (see Fig. 7). If we show that the modeled and observed label concentrations tend to converge over monthly timescales, we can argue that ignoring these short-term pools is not a first-order impediment to good estimates of allocation and growth. Other more subtle aspects of the problem could, however, have important implications for plot-scale and even global scale vegetation-soil ecosystem dynamics and feedbacks. For example, the labeled soil surface CO_2 efflux is a result from a combination of root respiration and heterotrophic respiration. The heterotrophic component can be supplied by fresh litter inputs or by root exudation of non-structural carbohydrate, which can be a significant fraction of net primary production in some systems (Högberg et al., 2010). The difference between root mortality and root exudation in terms of substrate quality, nutrient content, and interactions with soil microbial communities could be very significant, especially as integrated over long periods and under conditions of changing climate, changing atmospheric CO_2 concentration, and anthropogenic modifications to nutrient cycles.

Representing the existence and dynamics of short-term photosynthate storage pools in a model like CLM could also help to resolve the mechanisms relating nutrient mineralization and availability in soils with plant-microbe competition for available nutrients and the influence of nutrient uptake on leaf-scale photosynthesis. In addition to the shading treatments described here, other manipulations that would be useful to explore include elevated CO_2 during and/or after the labeling pulse, imposed nutrient limitations, and fertilization. Replicating these studies in other vegetation types would help to assess the generality of storage pool structure and function, and would support operational inclusion of these mechanisms in a global-scale model.

4.3 Implications for experimental design

Limitations identified in this first PiTS model-experiment interaction have already led to improvements in follow-on experiments. For new experiments in a nearby dogwood stand, additional observations include multiple treatments in different seasons, a collection of absolute destructive tree biomass at the end of the study (rather than highly uncertain 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, model parameters are being measured where 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. Additional effort is being devoted to characterizing the system prior to manipulation, including measurements of biomass, soil physical and soil biogeochemical states.

5 Conclusions

The point version of CLM4 was implemented, calibrated and evaluated against carbon and hydrology observations from a shading and labeling experiment in a stand of young loblolly pines. We found that a combination of parameters measured on-site and calibration targeting biomass, transpiration, and ^{13}C discrimination gave good agreement with pretreatment measurements, including independent evaluation metrics at the leaf-scale. We showed that the calibrated model captured the tree-scale and monthly temporal

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Our framework for functional unit testing provides for the isolation and evaluation of fundamental mechanisms and processes (functions and subroutines) in CLM or similar models. This ability makes it possible to compare model results with observations made during an experiment that would be very difficult, if near impossible, to do with ... [15]

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dynamics of a light-shade treatment as it influenced carbon and water fluxes. The calibrated model also captured the monthly time-scale carbon dynamics of a heavy-shade treatment, but persistently estimated low levels of transpiration for the heavy-shade treatment, while observed transpiration in that treatment remained nearly as high as for the light-shade. We have suggested several possible explanations for the discrepancy, but this remains a puzzling problem requiring further investigation.

Although the model lacks short-term photosynthate storage and transport mechanisms that are clearly present in the real plants, first-order monthly time-scale dynamics for carbon allocation and growth do not seem to suffer greatly. We used observations from the experiment to develop a conceptual model (hypothesis) of short-term photosynthate storage and transport, and suggested further studies that could be carried out to evaluate the generality of the hypothesized mechanisms. We suggested several research problems, which, if the proposed mechanism turns out to be generally valid, would benefit from model-experimental study in which the new mechanisms are incorporated into the model structure.

Acknowledgements. This work is supported by the US Department of Energy (DOE), Office of Science, Biological and Environmental Research. Oak Ridge National Laboratory is managed by UT-BATTELLE for DOE under contract DE-AC05-00OR22725.

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Table 1.

Parameter	Description	Units	Default	PRE_OPT	HS_MB
measured					
slatop	Top of canopy specific leaf area (SLA)	m^2/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	$\mu mol\ m^{-2}\ s^{-1}$	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

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

Table 2.

State variable	Units	Observed	PRE_STD	PRE_OPT	Bias reduction (%)
Leaf carbon	gC/m^2	[182,221]	419	209	96.55
Stem carbon	gC/m^2	[973,1220]	1455	1027	88.49
Root carbon	gC/m^2	488	859	408	78.44
Aboveground biomass	gC/m^3	[728,1758]	1645	1236	98.26
δ13C leaf	per mil	-27.99	-27.38	-27.49	18.03
δ13C phloem	per mil	-28.48	-27.38	-27.50	10.91
δ13C Root	per mil	-28.86	-27.36	-27.39	2.13
Sap flow	mm/day	2.40	3.70	2.37	97.85
Soil respiration	$\mu mol\ m^{-2}\ s^{-1}$	3.63	5.20	3.26	76.58

Captions of Tables and Figures

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 (ENF) 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.

Table 2. Pretreament state variables included in the optimization. Simulated values were obtained using the default parameters (PRE_STD) and the optimized parameters (PRE_OPT). The bias reduction (%) caused by the optimization is listed in the last

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column. In the case of leaf, root and aboveground biomass, we use allometric equations from multiple sources (Baldwin, 1987; Naidu et al., 1998; Vanlear et al., 1986) that went into producing a range. The bias calculation uses the mean of the range. For sap flow and soil respiration, daily observations were made, but the values represent a mean over the 25 pretreatment days over both LS and HS periods. δ^{13}C values represent observed and simulated values on the day before treatments began.

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 $^{13}CO_2$ (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

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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 CO$_2$ concentrations (Ci) and leaf temperatures (Tleaf) at the observed light (PAR) levels and the site's observed leaf nitrogen (Na). Three grey bars represent the mean ± 1 std dev of midday PAR levels under the light shade treatment (LS), heavy shade treatment (HS) and open field condition (OF).

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

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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 δ^{13}C (parts per thousand (‰)) of (a) leaf, (b) phloem, (c) bulk root and (d) soil surface efflux δ^{13}C for the light shade (LS, open circle) and heavy shade (HS, filled circle) pretreatment and treatment periods (± standard error (SE)). The modeled δ^{13}C values were calculated from the CLM simulated ^{13}C and ^{12}C variables and the reference standard (0.0112372) using the equation described in https://en.wikipedia.org/wiki/Δ13C. The $^{13}CO_2$ 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 δ^{13}C values for the light shade (open triangle) and heavy shade (filled triangle) treatments from Day 1 to Day 25.

Figure 7. Conceptual model of label transport, assuming a constant velocity (V) of phloem stream with a cross-sectional area for the phloem pathway that varies as a function of ongoing photosynthetic rate. Cross-sectional area is conceptualized here as a varying number of similar phloem elements, with white elements in an active state, and dark elements inactive. The experimental case with a higher photosynthetic rate for the LS treatment and lower photosynthetic rate for the HS treatment is illustrated. Flux from roots (FR) includes root respiration, root exudation, and turnover of root tissue. The entire label is assumed to exit the leaf and enter the active phloem stream, at a rate that is independent of the ongoing rate of photosynthesis, as observed in the experiment.

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The model predicted exponential growth in all biomass pools was observed during the 8 years

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Compared to the standard CLM results, C stocks of the simulation with optimized parameters were lower

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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. The persistently larger difference between simulated and observed assimilation at PAR of approximately 500 µmol m^{-2} s^{-1} is a consequence of the assumption in CLM4 of carboxylation being limited by a single factor (i.e, the calculation of the limiting carboxylation rate as the absolute minimum value of the RuBisCO-, RuBP regeneration- and TPU-limited rates of carboxylation) (Harley and Sharkey, 1991). Assuming co-limitation between the individually limited rates of carboxylation, a smoother transition between limiting factors and an improved fit with observations at the transition point of approximately 500 µmol m^{-2} s^{-1} can be obtained by solving for the minimum carboxylation rate using coupled quadratics as in Collatz et al. (1991).

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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).

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The model displayed almost no short-term variability in stem carbon - the model does not represent stem swelling and shrinking with water status.

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The observed foliar $\delta^{13}C$ 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 $\delta^{13}C$ of LS and HS were similar by Day 8, and $\delta^{13}C$ 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 ^{13}C 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 $\delta^{13}C$ 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 δ^{13}C 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 ^{13}C concentrations. The model does capture the fact that LS δ^{13}C declines faster than the high shade δ^{13}C. In the simulation, this occurs in the LS case because of the dilution of the δ^{13}C 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 δ^{13}C 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) δ^{13}C under either shade treatment and little difference between LS and HS. In both simulations, phloem δ^{13}C changed little compared to observations, through the shading period (Fig. 6b). As with leaf δ^{13}C, phloem δ^{13}C 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 δ^{13}C.

There was no consistent shade treatment effect in the observed δ^{13}C 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 δ^{13}C values in the fine-root pool were still higher than the background δ^{13}C levels, especially in the LS treatment. The model overestimated the background bulk root δ^{13}C for the pretreatment period by 2‰. As with foliar and phloem δ^{13}C, after Day 1 bulk root δ^{13}C values remained nearly stable in the

HS simulation and slightly declined in the LS simulation, again representing dilution by new photosynthate.

The simulated $\delta^{13}C$ efflux 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 $\delta^{13}C$ values occurring on Day 3 for LS and Day 4 for HS. Observed $\delta^{13}C$ of soil CO_2 efflux decreased exponentially after the peak under both treatments. The model, on the other hand, simulated decreases of $\delta^{13}C$ soil CO_2 efflux to near pre-treatment 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.

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Pretreatment results

The optimized

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In addition to the importance of optimized 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.

4.2 Treatment results

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 that improvement in CLM process representation is needed to capture realistic site hydrology (Li

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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. 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) is 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.,

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In contrast with observations, there was no difference in simulated HS and LS soil respiration prior to the shading (Fig. 5b). After examining the simulated respiration fluxes, we determined the lack of pretreatment difference in simulated soil respiration and the small increase in post-treatment simulated soil respiration under LS is mainly a consequence of the higher growth respiration from coarse and fine roots that results from higher GPP and allocation to these pools in the LS conditions. This phenomenon might also explain the smaller post-treatment difference between observed HS and LS soil respiration, with higher root respiration under LS narrowing the pretreatment difference between HS and LS soil respiration.

The model’s carbon allocation to the stem may also be less sensitive to short-term variation in environmental conditions than whatever contribution to observed (allometrically defined) variations in stem biomass are a result of actual stem growth and respiration (Fig. 5a). 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 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 ^{13}C enrichment in autotrophic and heterotrophic C fluxes. 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 soil CO_2 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 model's allocation to roots and the root's utilization of that carbon needs attention.

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future model development and 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

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is best done as part of the model design process.

There were some limitations of this first PiTS observational dataset that have implications for subsequent efforts. Future experiments in a

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will address several issues based on knowledge gained from the PiTS 1 model-experiment efforts, including physical separation of treatments. New

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Our framework for functional unit testing provides for the isolation and evaluation of fundamental mechanisms and processes (functions and subroutines) in CLM or similar models. This ability makes it possible to compare model results with observations made during an experiment that would be very difficult, if near impossible, to do with even a site-scale implementation of a LSM such as PTCLM. These models quite reasonably focus on, and generate output for, aggregate whole-stand properties such as stand-scale net ecosystem exchange and evapotranspiration. However, many experimental observations are at finer scales involving individual components of the stand or ecosystem (e.g., individual leaves). As used in this study, the functional unit testing allows for model evaluation at the empirically accessible scales of experimental field observations (Fig. 3b).

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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., Ball-Berry stomatal conductance slope and Ball-Berry stomatal conductance intercept), 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, it is not able to reproduce the observed patterns of allocation revealed by the ^{13}C labeling experiment. 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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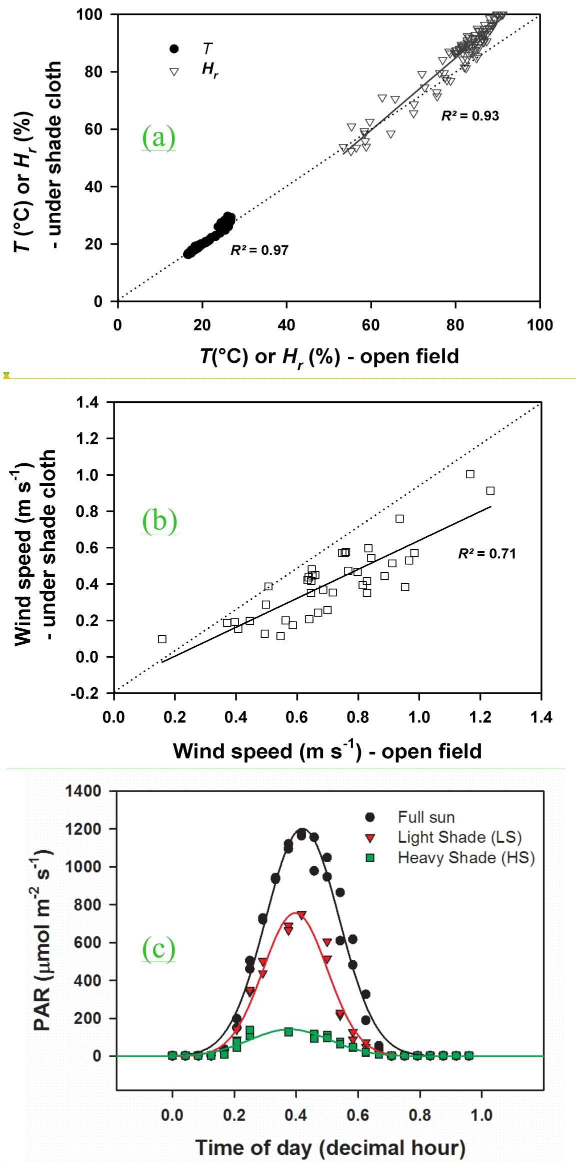
measured					
slatop	Top of canopy specific leaf area	m^2/gC	1.00E-02	1.02E-02	1.02E-02
dsladlai	Change in SLA through per unit LAI	gC^{-1}	1.25E-03	0	0
leafcn	leaf C:N ratio	gC/gN	35	50	50
optimized					
mp	Ball-Berry stomatal conductance slope	none	6	5.59	71.3
bp	Ball-Berry stomatal conductance intercept	$\mu mol\ m^{-2}\ s^{-1}$	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



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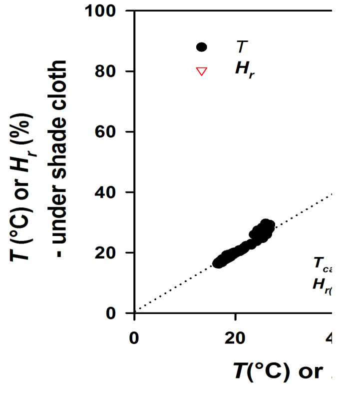

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Figure 1 (a) Air temperature (T, °C), relative humidity (Hr, %) and (b) wind speed (u, m s^{-1}) under the shade cloth at the top of the canopy compared with open field measurements at 2 m height; (c) Typical diurnal patterns of photosynthetically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

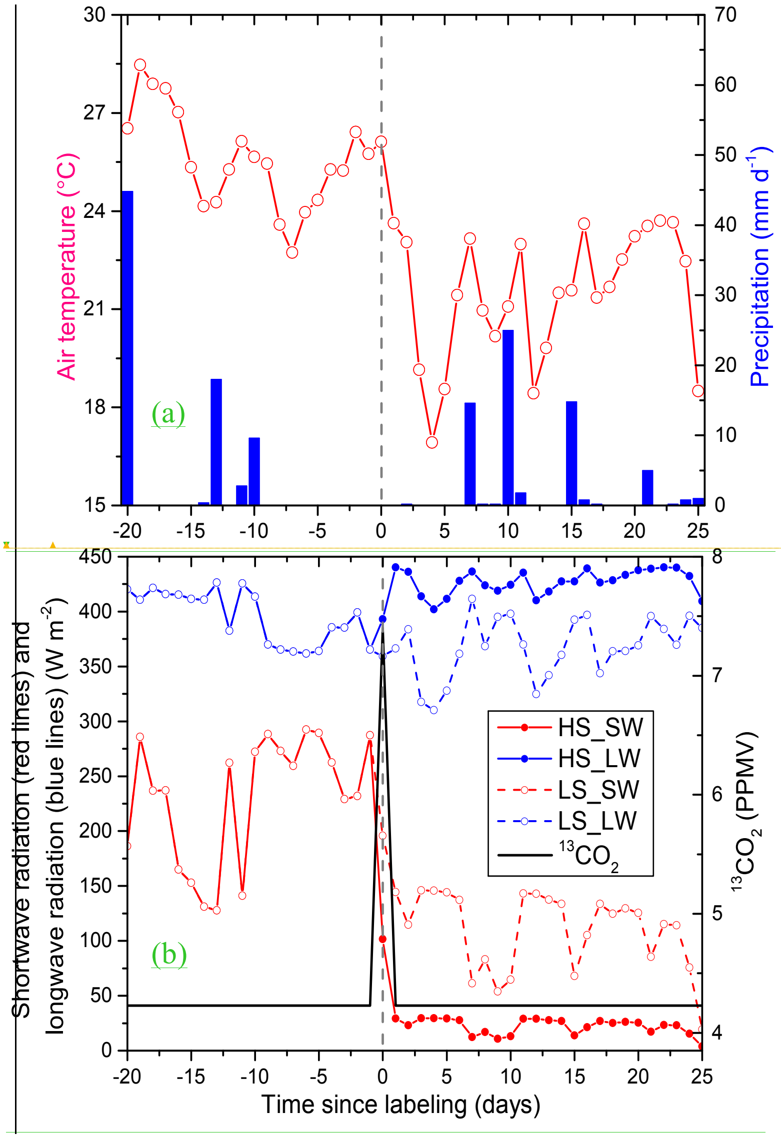

Figure 2 (a) Daily air temperature (°C) and precipitation (mm d^{-1}) for the pretreatment and treatment of light shade (LS) and heavy shade (HS) (Day -20 to 25), (b) change in daily atmospheric long wave radiation (LW, W m^{-2}), short wave

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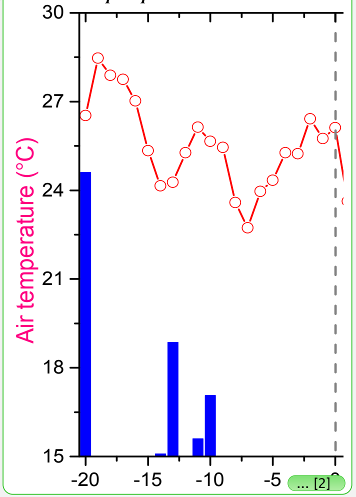

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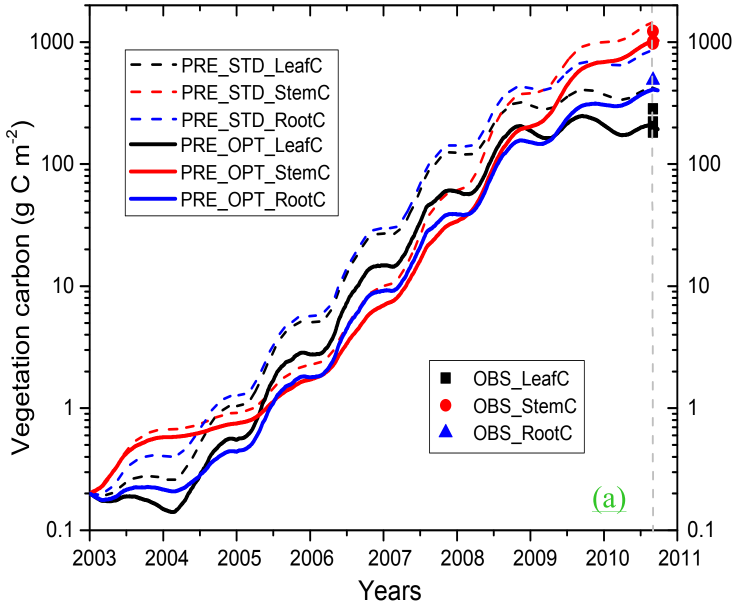
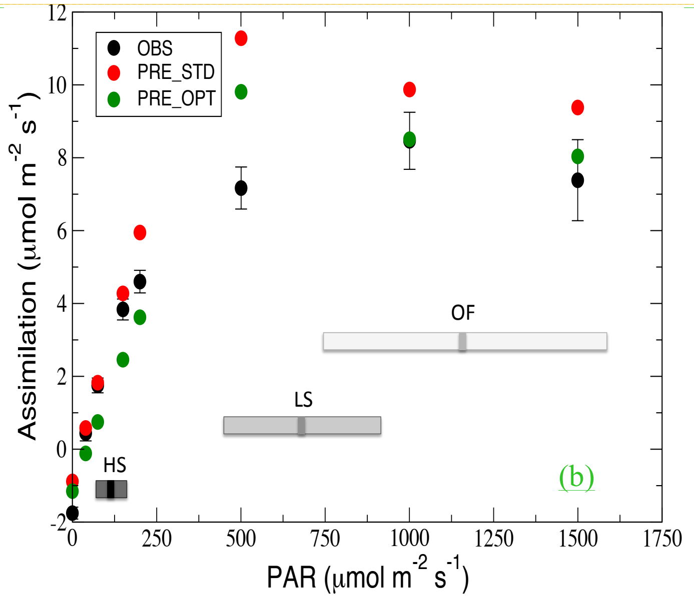
radiation (SW, W m^{-2}) and $^{13}CO_2$ (PPMV) prior to and after exposure to shade treatments. Dashed gray line represents the starting day of the treatment.





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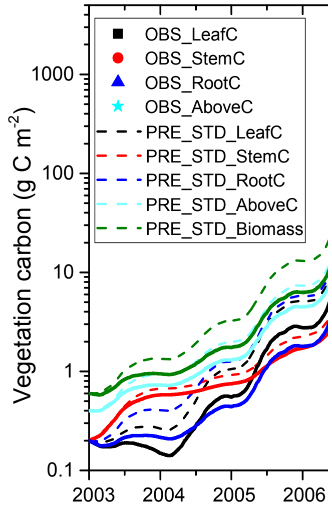

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Figure 3 (a) CLM simulated change of leaf carbon (PRE_STD_LeafC), stem carbon (PRE_STD_StemC) and root carbon (PRE_STD_RootC) with default parameters, and change of those (PRE_OPT_LeafC, PRE_OPT_StemC and PRE_OPT_RootC) simulated with optimized parameters 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 CO$_2$ concentrations (Ci) and leaf temperatures (Tleaf) at the observed light (PAR) levels and the site's observed leaf nitrogen (Na). Three grey bars represent the mean ± 1 std dev of midday PAR levels under the light shade treatment (LS), heavy shade treatment (HS) and open field condition (OF).

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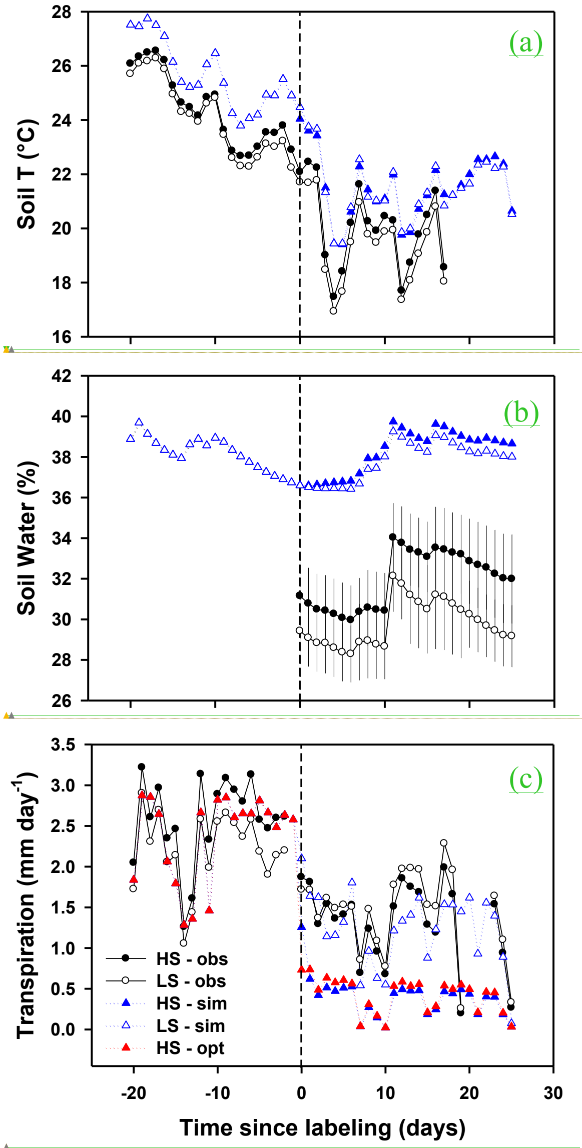

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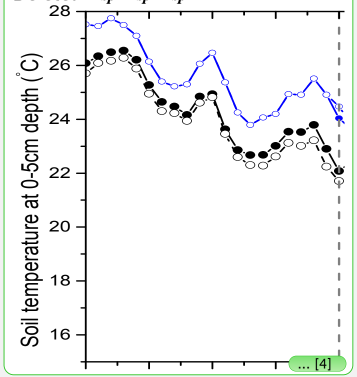

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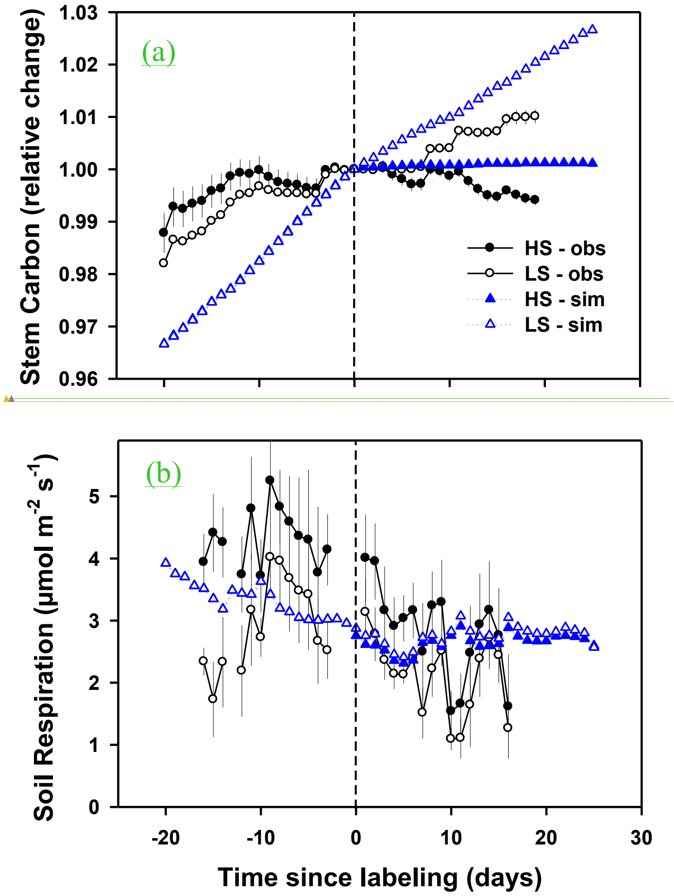
Figure 4 (a) Observed (obs) and CLM simulated (sim) daily soil temperature at 0-5cm depth (standard deviation, *SD* = 0.6-1.4 °C), (b) volumetric soil water content at 15-95cm depth (±*SD*) and (c) the transpiration before and after initiation of light shade (LS) or heavy shade (HS) treatments (*SD* = 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.



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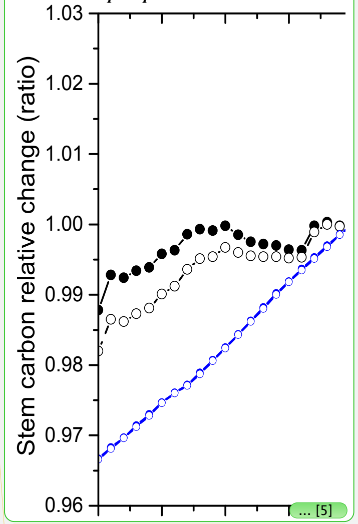

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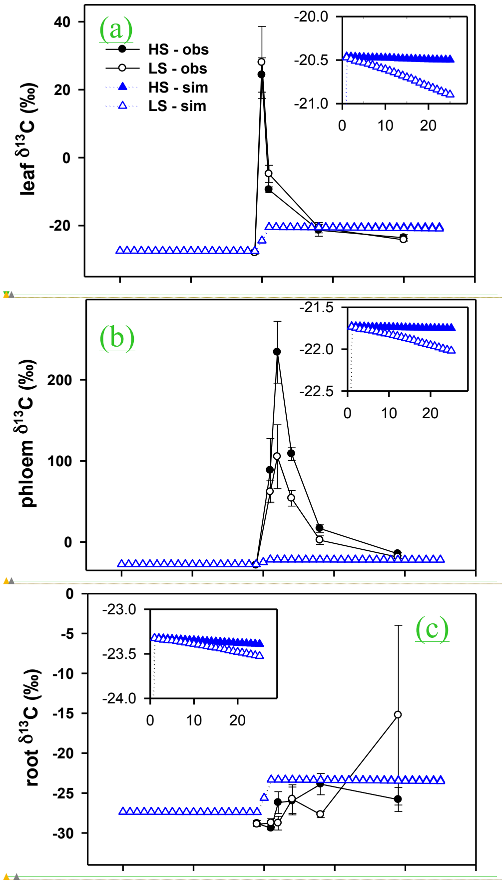
Figure 5 (a) Observed (obs) and CLM simulated (sim) daily stem carbon relative to day 0 (±*SD*), and (b) soil respiration prior to and after exposure to light shade (LS) and heavy shade (HS) treatments (±*SD*). Both observed and simulated stem carbon were normalized to 1 at Day 0. The simulated soil 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.



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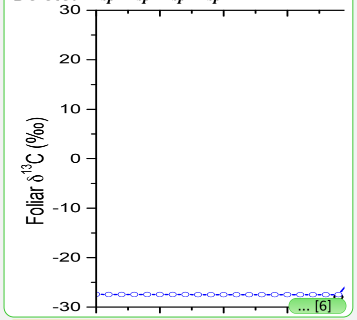

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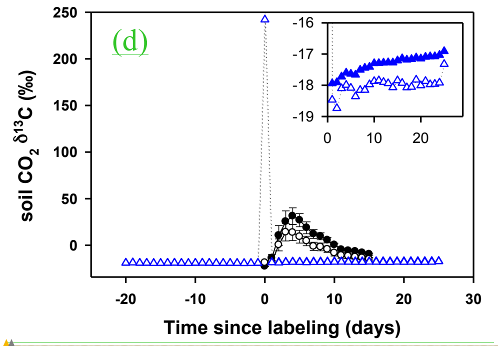

Figure 6 (a) Observed (black) and CLM simulated (blue) change in δ^{13}C (parts per thousand (‰)) of (a) leaf, (b) phloem, (c) bulk root and (d) soil surface efflux δ^{13}C for the light shade (LS, open circle) and heavy shade (HS, filled circle) pretreatment and treatment periods (± standard error (SE)). The modeled δ^{13}C values were calculated from the CLM simulated ^{13}C and ^{12}C variables and the reference standard (0.0112372) using the equation described in https://en.wikipedia.org/wiki/Δ13C. The ^{13}CO$_2$ 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 δ^{13}C values for the light shade (open triangle) and heavy shade (filled triangle) treatments from Day 1 to Day 25.

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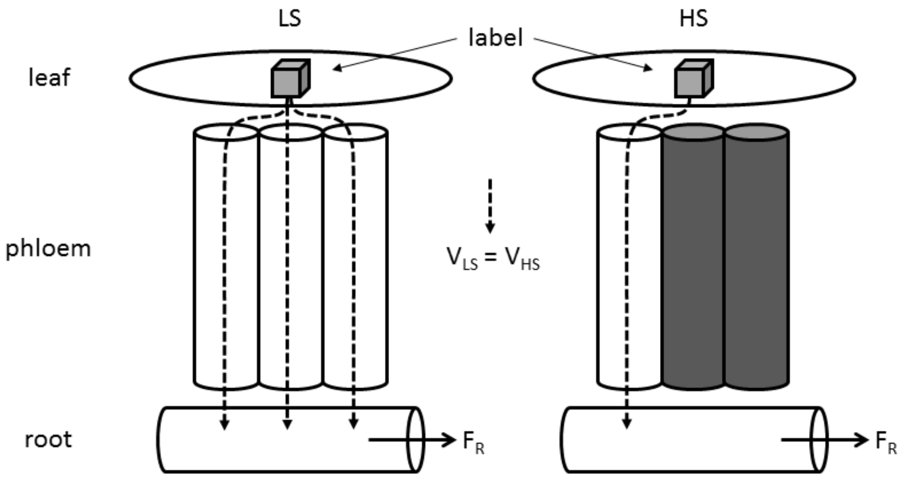

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Figure 7. Conceptual model of label transport, assuming a constant velocity (V) of phloem stream with a cross-sectional area for the phloem pathway that varies as a function of ongoing photosynthetic rate. Cross-sectional area is conceptualized here as a varying number of similar phloem elements, with white elements in an active state, and dark elements inactive. The experimental case with a higher photosynthetic rate for the LS treatment and lower photosynthetic rate for the HS treatment is illustrated. Flux from roots (FR) includes root respiration, root exudation, and turnover of root tissue. The entire label is assumed to exit the leaf and enter the active phloem stream, at a rate that is independent of the ongoing rate of photosynthesis, as observed in the experiment.

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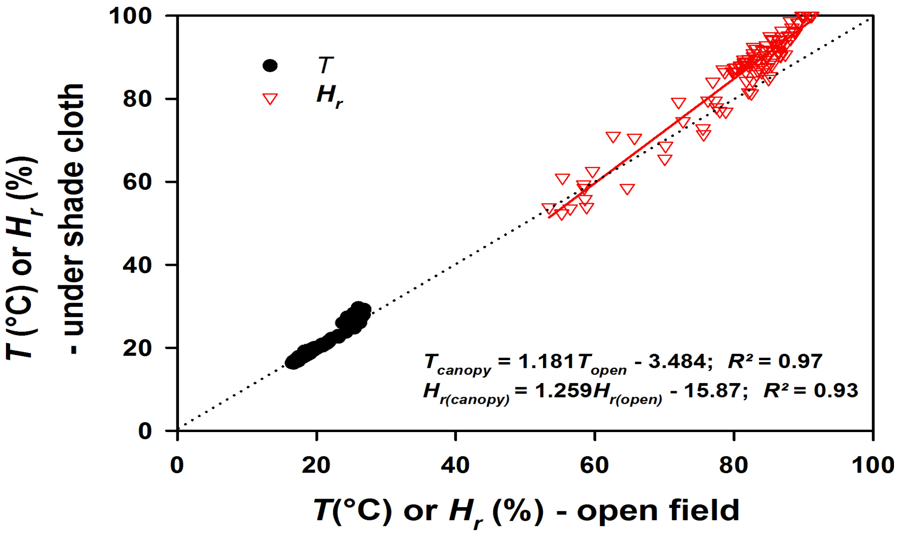
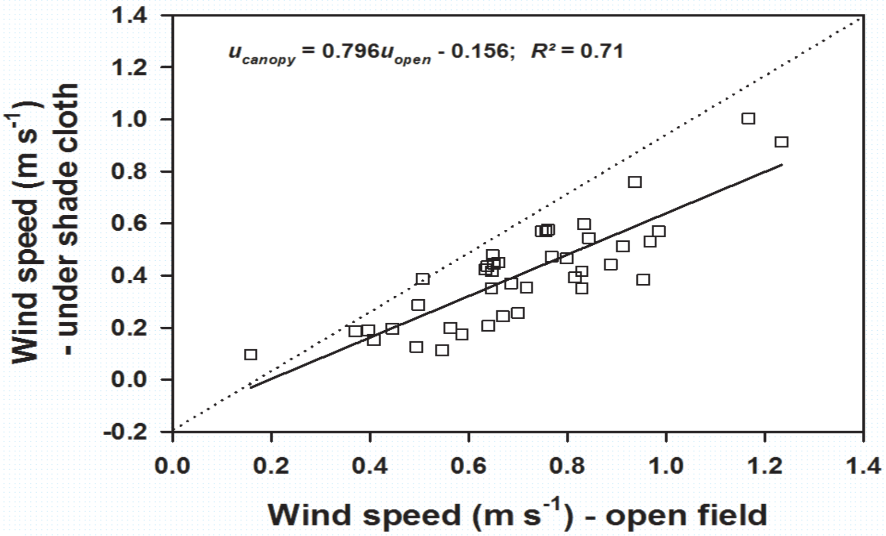
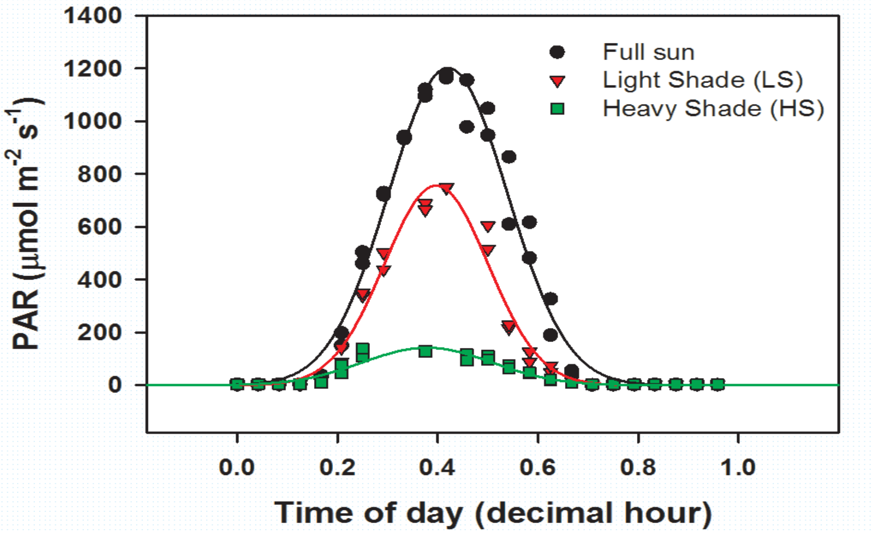
(a)



(c) (b)





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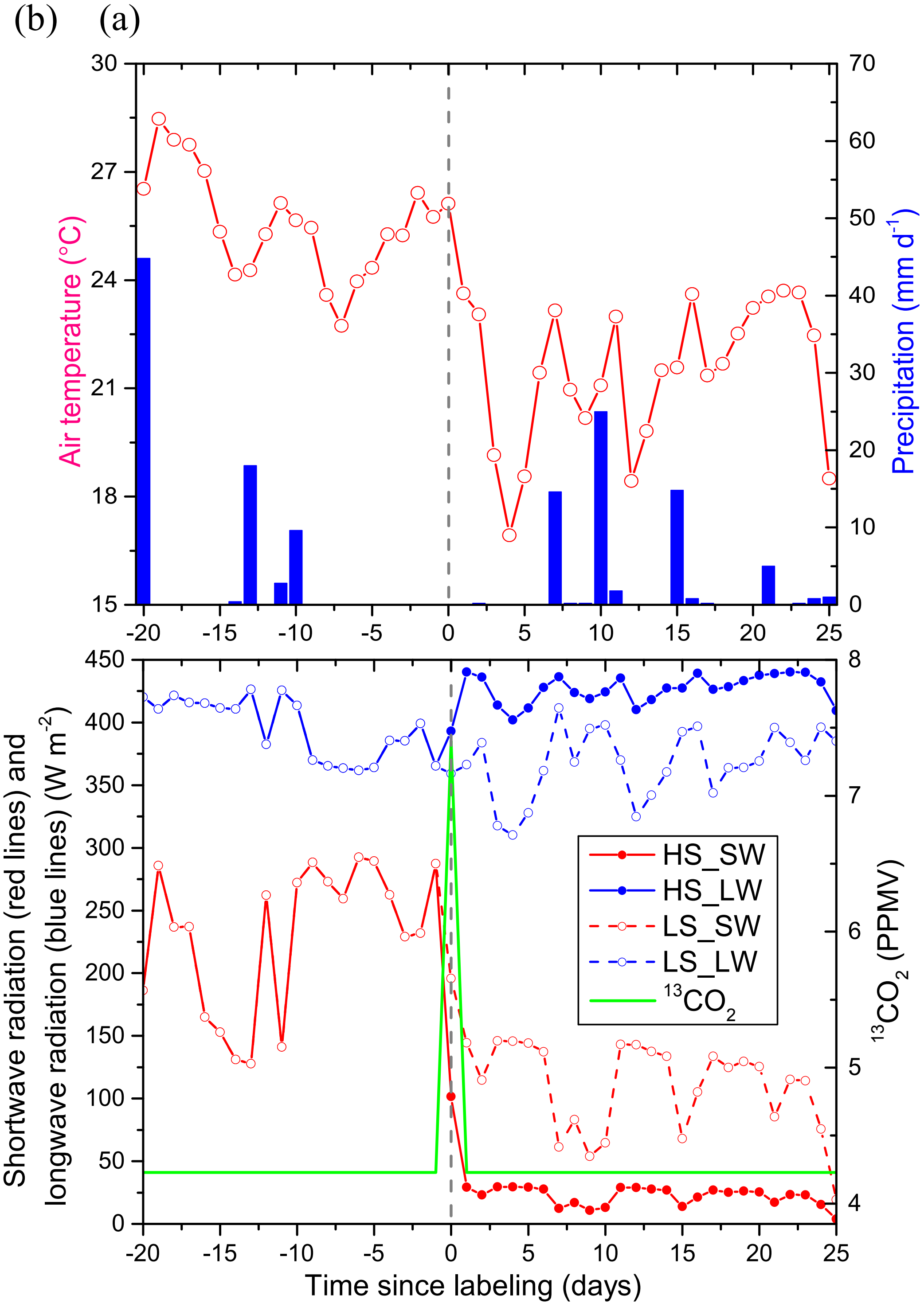

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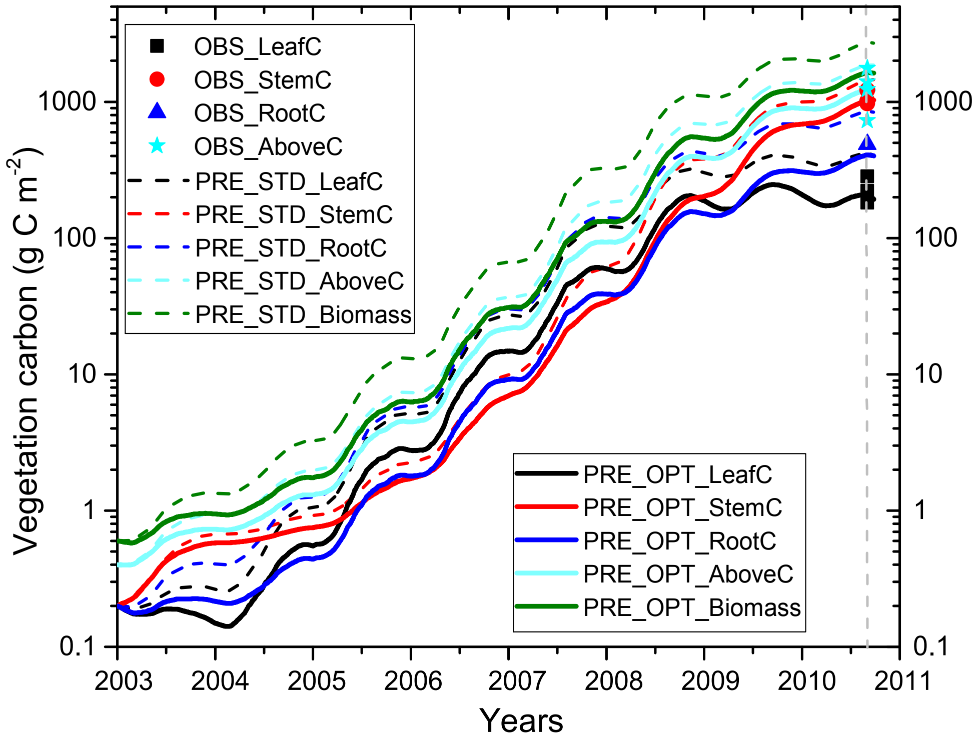

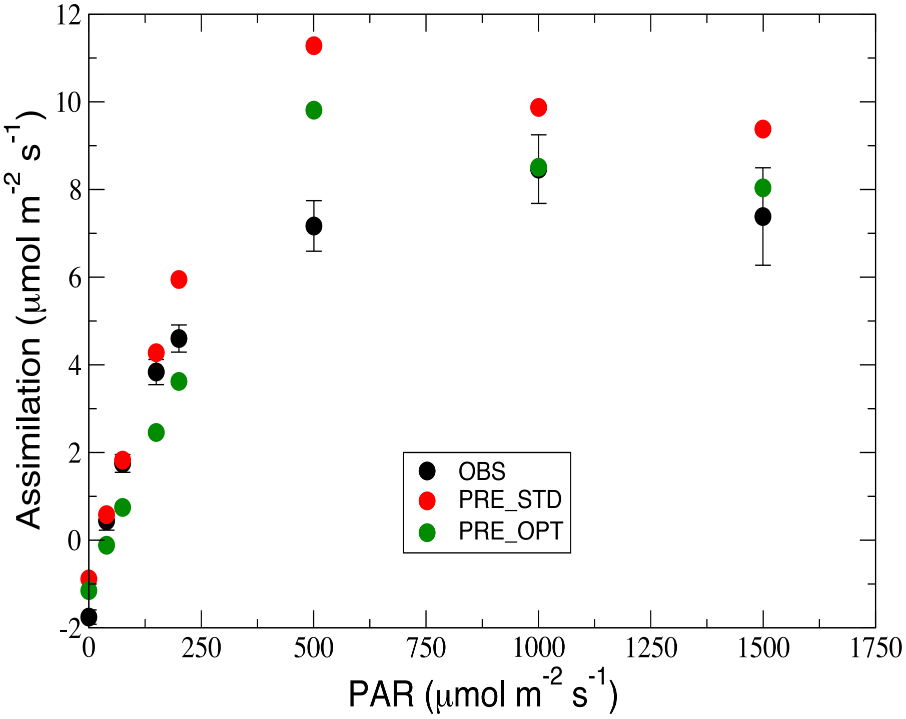

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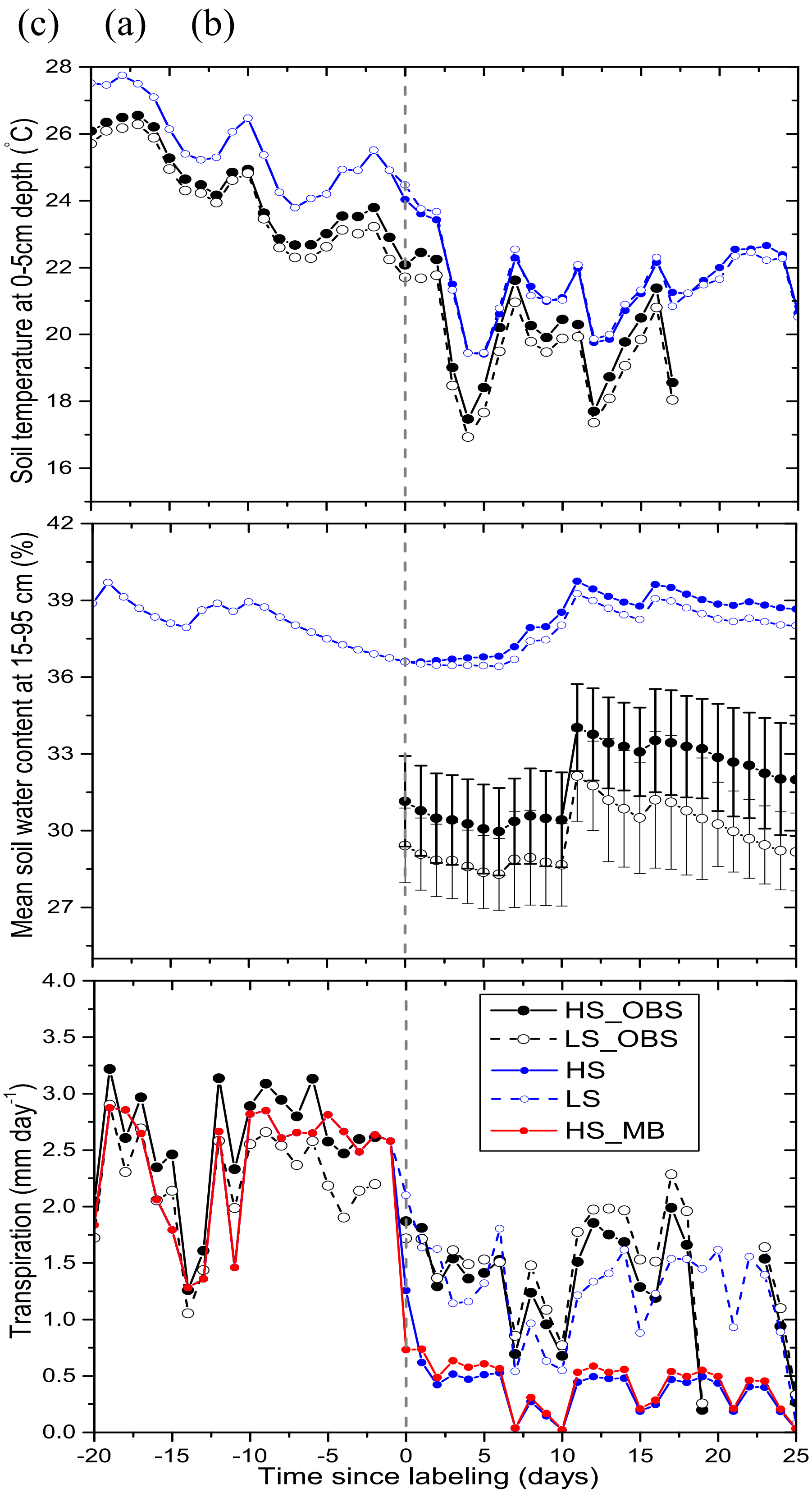

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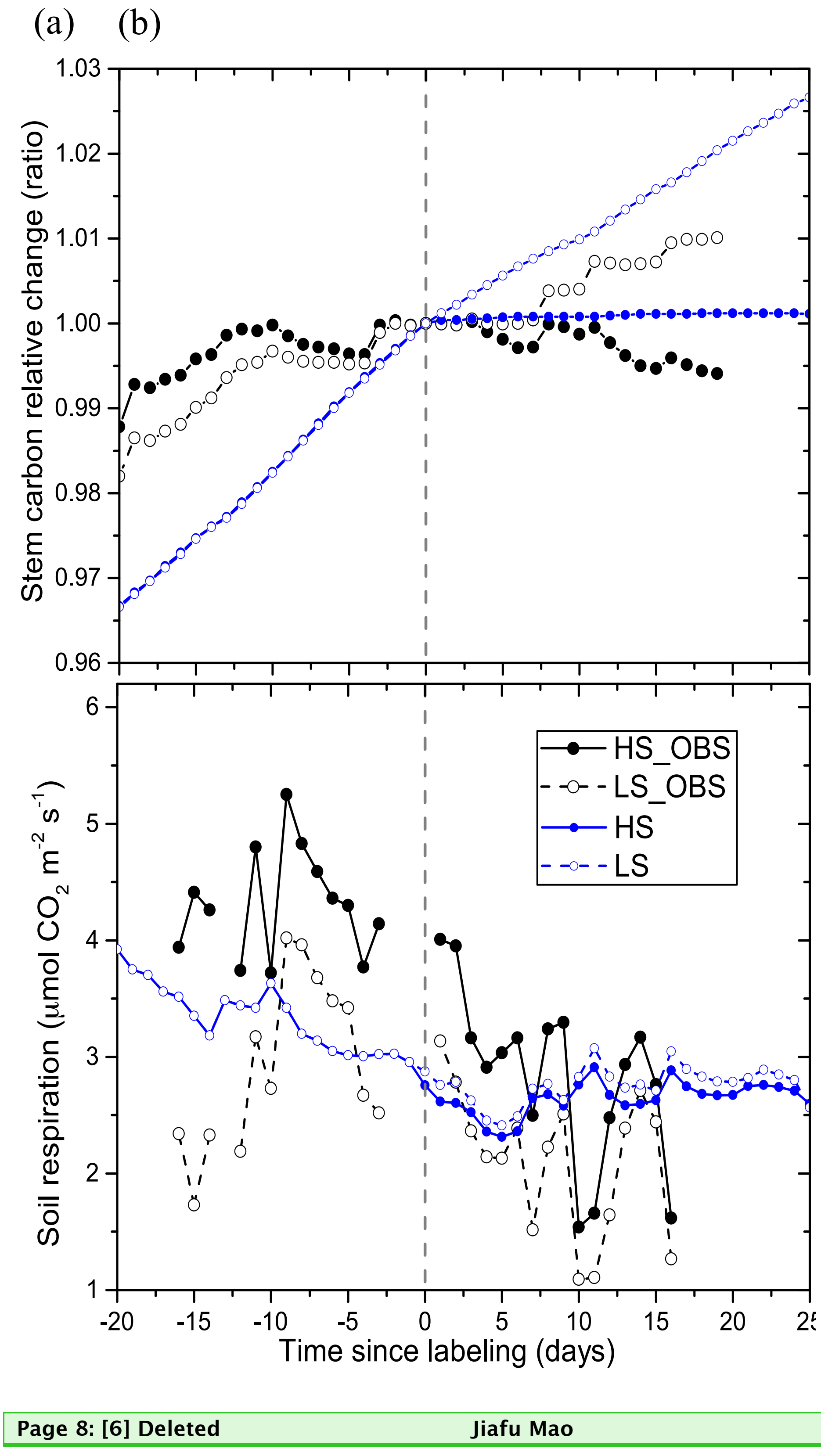

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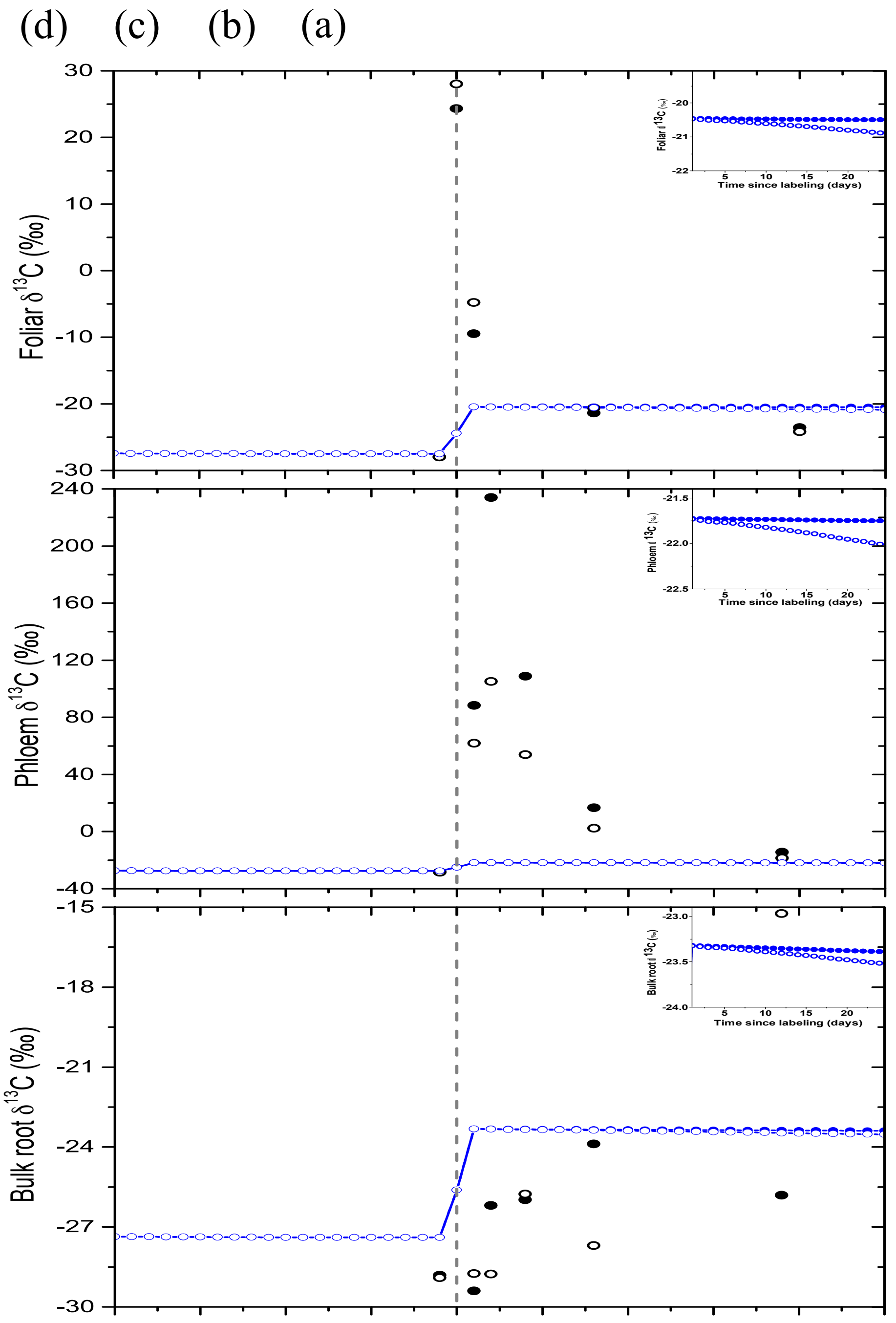

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(c)
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0
-10
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Foliar δ13C (‰)
-20
-21
-22
5
10
15
20
Time since labeling (days)
Phloem δ13C (‰)
240
200
160
120
80
40
0
-40
Phloem δ13C (‰)
-21.5
-22.0
-22.5
5
10
15
20
Time since labeling (days)
Bulk root δ13C (‰)
-15
-18
-21
-24
-27
-30
Bulk root δ13C (‰)
-23.0
-23.5
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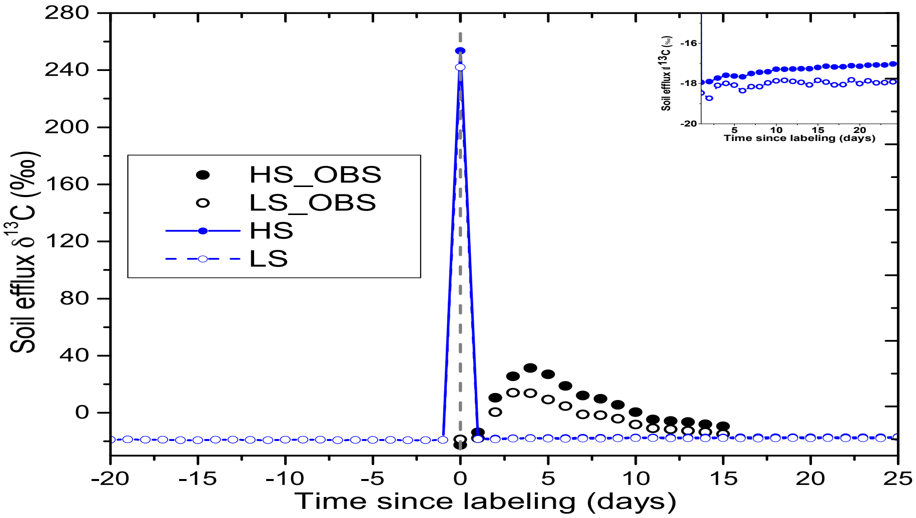
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Time since labeling (days)
HS_OBS
LS_OBS
HS
LS
Soil efflux δ13C (‰)
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-20
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Time since labeling (days)