Letter of Responses

Authors' note: The original reviewers' comments are *in italic and colored blue*, and our responses follow. All page/line numbers indicated in the responses are those in the marked-up revision. In addition, a clean version of the revised manuscript has also been provided.

Reviewer 1 (Dr. W. Wieder)

Liang and coauthors present a nice study exploring sensitivities in the E3SM land model to changes in the calculation of soil water potential and subsequently to parametric changes related to plant physiology. They compare simulated results to observations from the MOFLUX site, focusing on carbon fluxes (GPP and soil respiration, SR).

There are a host of changes suggested that generally improve agreement with observed results, but in general it's hard to follow what changes are most important for the improvements. I appreciate the need to keep text and display items simple & digestible for readers, but a bit more complexity would help shed light on the factors responsible for the site-level improvements in the model made here. For example, it looks like the modified soil water potential scheme (Hanson, I think), provides a better fit to GPP, SR and soil moisture (Figs. 2-5), but it remains unclear if the modifications are significantly better (or different) from the Clapp & Hornberger scheme that's been tuned to local edaphic characteristics? It's not that surprising that the parameterization for a global model would not be a good fit to local results, so does the model just need tuning for site-level runs, or are underlying physics and assumptions in the Hanson scheme fundamentally superior to another approach? Addressing this question matters if the long-term aim of this work is to document changes made to ELM from CLM4.5.

Response: We greatly appreciate the valuable comment. Particularly interesting is the question *"if the modifications are significantly better (or different) from the Clapp & Hornberger scheme that's been tuned to local edaphic characteristics"*. In the revised manuscript, we compared the simulated gross primary production (GPP) and soil respiration (SR) when using the Hanson model and the calibrated Clapp & Hornberger model. Generally, both the Hanson model and the calibrated Clapp & Hornberger model improved the simulation of GPP and SR in the E3SM Land Model version 0 (ELMv0), in comparison with the default run with the uncalibrated Clapp & Hornberger model (Fig. S8 and also see below). The ELMv0 with the Hanson model consistently produced higher GPP and SR than that with the calibrated Clapp & Hornberger model. In comparison with the observations, the modelled SR generally fell within the 1 sigma (i.e., standard deviation) range of observations, by using both the Hanson model and the calibrated Clapp & Hornberger model. However, the modelled GPP with the calibrated Clapp & Hornberger model was lower than the observations. Given the order of the goodness-of-fit of the soil water potential (SWP)-volumetric water content (VWC) relationship was default Clapp & Hornberger model < calibrated Clapp & Hornberger model < calibrated Hanson model (revised Table 1 and also see below), these new results further support our conclusion that better representations of SWP can improve the simulations of carbon processes (i.e., GPP and SR here).

In the revised manuscript, we added a new supplementary figure (i.e., Fig. S8) and a paragraph in the text to compare simulations with the Hanson model and the calibrated Clapp & Hornberger model (page 12, lines 14 – 24):

"Moreover, we also explored whether the calibrated Clapp & Hornberger model can lead to similar improvements with the Hanson model (Fig. S8). Generally, both the Hanson model and the calibrated Clapp & Hornberger model improved the simulation of GPP and SR in the ELM, in comparison with the default run (Fig. S8). The ELMv0 with the Hanson model consistently produced higher GPP and SR than that with the calibrated Clapp & Hornberger model. In comparison with the observations, the modelled SR generally fell within the 1 sigma (i.e., standard deviation) range of observations, by using both the Hanson model and the calibrated Clapp & Hornberger model. However, the modelled GPP with the calibrated Clapp & Hornberger model was still lower than the observations. Given the order of the goodness-of-fit of the SWP-VWC relationship was default Clapp & Hornberger model < calibrated Clapp & Hornberger model < calibrated Hanson model (Table 1), these results further support the conclusion that better representations of SWP can improve the simulations of carbon processes. Therefore, throughout the remainder of this manuscript, we used the Hanson model to represent the SWP-VWC relationship."

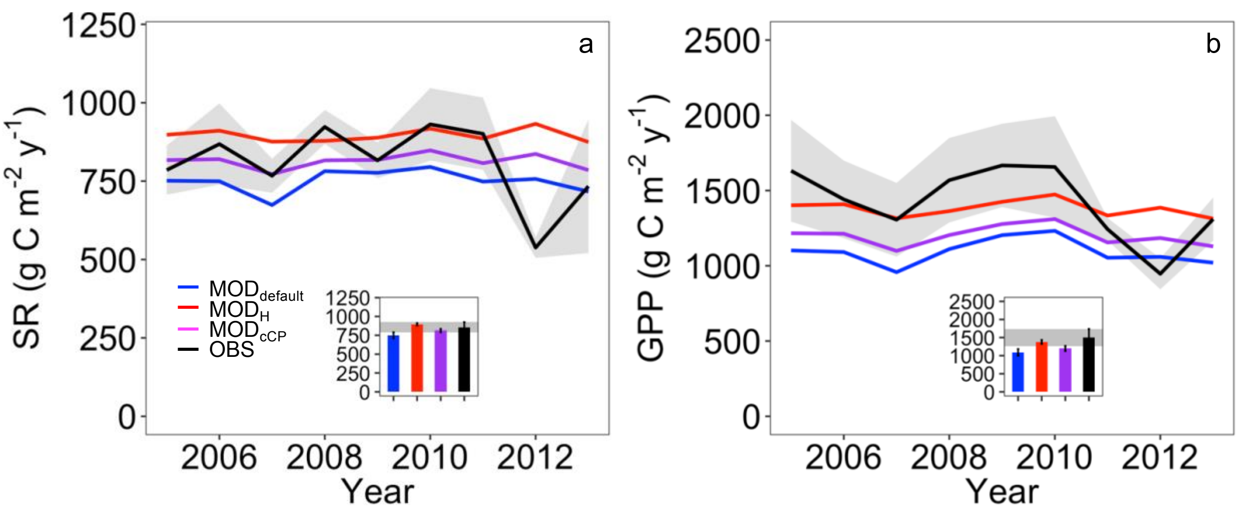

Figure S8: Annual soil respiration (SR) and gross primary production (GPP). Blue lines are the ELMv0 simulations with default parameters ($MOD_{default}$), red lines with the soil water potential improved using the calibrated Clapp & Hornberger model (MOD_{cCP}), and purple lines with the soil water potential improved using the Hanson model (MOD_{H}). Black lines and grey area are the observed (OBS) mean and 1 sigma range, which were calculated from eight field replications for SR, and from three different net ecosystem exchange partitioning methods for GPP. The inserted bar plots are mean annual average ± 1 sigma across 2005-2011.

The reviewer also asked *"are underlying physics and assumptions in the Hanson scheme fundamentally superior to another approach"*. The short answer is no. Although different approaches for soil water retention curve may have different underlying physics and assumptions, pragmatic models are those which have been well calibrated/parameterized with empirical data. Since the default ELMv0 simulated the SWP poorly at the MOFLUX site (Fig. 3b), one important question we asked in this study was whether better representation of SWP in the model would improve the simulations of carbon processes. To improve the SWP simulation as much as possible, our effort was not limited to tuning the Clapp & Hornberger model since we did not know whether the tuned Clapp & Hornberger model would be good enough to answer the question. Instead, we evaluated a series of soil water retention curve models popularly used in the literature to derive the best-fit model using root-mean-square-error (RMSE) and Akaike Information Criterion (AIC) as suggested by the reviewer's other comments (revised Table 1 and also see below). The Hanson model performed the best, showing the smallest RMSE and AIC values. Both the modelled annual fluxes of GPP and SR fell within the 1 sigma range of observations when using the Hanson model, but not with the calibrated Clapp & Hornberger model as shown in Fig. S8 and above. Thus, we used the Hanson model for all further analyses. In the reminder of this response letter and the manuscript, the improved SWP was simulated using the Hanson model if not otherwise specified, and all changed ELMv0 simulations were compared to the default simulations with the default Clapp & Hornberger model.

Table 1. Root-mean-square-error (RMSE) and Akaike Information Criterion (AIC) of different models in simulating the SWP-VWC relationship for the soil in the MOFLUX site at two depths: 0 to 30 cm and below 30 cm.

	< 30 cm		> 30 cm	
Model	RMSE	AIC	RMSE	AIC
Clapp & Hornberger (default ELMv0)	4.25	157.82	1.33	18.51
Brooks & Corey	3.91	151.05	1.13	13.51
Clapp & Hornberger (calibrated)	0.53	-61.03	0.51	-23.43
Fredlund & Xing	0.51	-63.15	2.43	47.13
Hanson	0.41	-86.07	0.34	-38.98
van Genuchten	0.50	-65.53	0.36	-36.61

Although it needs further exploration as to whether the Hanson model performs the best on the regional and global scales, the default Clapp & Hornberger model used in the ELMv0 performs poorly in simulating SWP on the global scale (See below), which may significantly impact the biogeochemical simulations. In a different (but related) project, we tested the simulated SWP by the default Clapp & Hornberger model used in the ELMv0 against 6928 data points of paired measurements of SWP and VWC across different soil types and ecosystems. Results showed that the default Clapp & Hornberger model used in the ELMv0 was not able to reproduce the observed SWP (see Fig. R1 below). It remains unclear which model will perform best in describing the SWP-VWC relationship on the global scale. More work will be needed to explore the issue, which is beyond the scope of this manuscript.

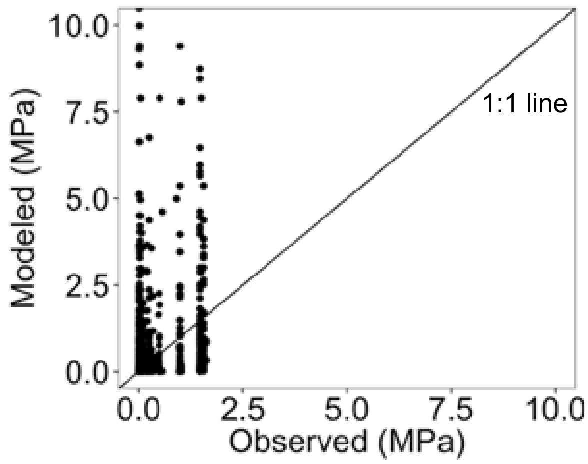

Figure R1: Comparison of observed and simulated soil water potential (-MPa) across different soil types and ecosystems by the default Clapp & Hornberger model in the ELMv0.

Similarly, how important are the suggested parameter changes for capturing the annual cycle of LAI and C fluxes vs. changes to the soil moisture scheme (Fig. 6). Stepping through these changes sequentially in the text and display items will clarify the source(s) of the improvements.

Response: The reviewer provided a great suggestion. Thanks to the reviewer's other suggestion, we are able to more clearly show the importance of the parameter changes and the improved SWP by plotting the mean annual cycle (± 1 sigma) of LAI, GPP and SR (revised Fig. 4 and also see below). With the revised figure, we can step through the changes. Results showed that the ELMv0 with both the default and improved SWP by the Hanson model overestimated the maximum LAI (Fig. 4a). The parameter adjustments significantly reduced the maximum LAI to better match the observations (Fig. 4a). The parameter changes further increased the simulated GPP and SR during the peak growing season, in addition to the improvement by the adjusted SWP (Fig. 4b, c). However, all modifications of the ELMv0 still overestimated SR during the non-growing season, as discussed (previously) in Section 4.2.

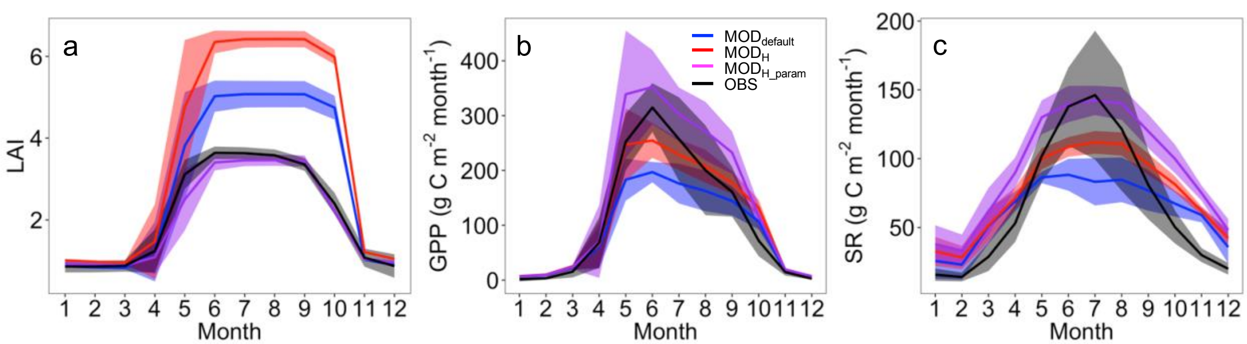

Figure 4 The annual mean cycles of leaf area index (LAI), gross primary production (GPP) and soil respiration (SR). OBS: observation; $MOD_{default}$: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement by the Hanson model; MOD_{H_param}: model output after soil water potential improvement by the Hanson model and parameter adjustments.

In the revised manuscript, we revised the text accordingly to show the effect of the parameter changes on the simulations of LAI, GPP and SR (page 10, lines 6 – 12):

"Results showed that the ELMv0 with both the default and improved SWP by the Hanson model overestimated the maximum LAI (Fig. 4a). The adjustment of the aforementioned five parameters (Table 2) significantly reduced the LAI to within a more reasonable range (Fig. 4a). The parameter changes further increased the simulated GPP and SR during the peak growing season, in addition to the improvement by the adjusted SWP (Fig. 4b, c). However, all modifications of the ELMv0 still overestimated SR during the non-growing season, resulting in significant overestimation of annual SR fluxes (Fig. S5a). After the parameter adjustments, the annual GPP flux was still within the observed range (Fig. S5b)."

Finally, although the authors claim that improving SWP directly improved soil respiration estimates, it's not clear if this is a direct effect of soil moisture on soil respiration, or merely reflective of the larger plant and soil C stocks simulated as a result of having higher GPP. Concurrently presenting changes to ecosystem C stocks and the soil moisture effect on GPP and heterotrophic respiration (btran and w_scalar, respectively in CLM4.5) will help clarify how / why improvements were made.

Response: We appreciate the insightful comment. The second reviewer had a similar concern. We agree with the reviewers that concurrently presenting changes in ecosystem carbon stocks and the soil moisture effect on GPP (btran) and heterotrophic respiration (ξ_W in equation 9) will help clarify how improvements were made. In the revised manuscript, we analyzed the changes in btran, ξ_W and soil organic carbon (SOC) (Fig. S2-S3 and also see below). The improved soil water scheme using the Hanson model increased both btran and ξ_W during the peak growing season, and reduced ξ_W during the non- growing season (Fig. S2). The change in ξ_W was generally consistent with that of SWP (Fig. 3b). While the model simulated SOC with different soil water schemes generally fell within the wide range of observations, the improved SWP simulations increased SOC stocks, matching the reviewer's expectation (Fig. S3). These results, combining with previous results (the original Fig. 4, which was moved as Fig. S1 in the revision as suggested by the reviewer's other comment), indicate that the improved soil respiration by SWP was a joint result of changes in GPP, SOC stocks and the moisture modifier of heterotrophic respiration.

In the revised manuscript, we added these new figures, presented the results and discussed details in the text.

Page 8, lines 1 – 6: *"The changes in annual SR and GPP (i.e., the differences between before and after the improved SWP simulation using the Hanson model) showed a linear relationship (Fig. S1). In addition, the improved soil water scheme using the Hanson model increased both the moisture modifiers of GPP and heterotrophic respiration (i.e., btran and* ξ_W*) during the peak growing season, and reduced* ξ_W *during the non-growing season (Fig. S2). While SOC when simulated by the model with different soil water schemes generally fell within* *the wide range of observations, the improved SWP simulations using the Hanson model increased SOC stocks (Fig. S3).”*

Page 11, lines 3 – 14: *“Constraining the SWP-VWC relationship with site-specific data and using the Hanson model instead of the ELMv0 default model (Fig. 1) significantly improved the model representation of SWP (Fig. 3) and annual SR (Fig. 2a). The improvements in model fits were due to changes in GPP, SOC stocks, and the moisture modifier on heterotrophic respiration (Figs. S1 – S3). First, the default ELMv0 underestimated GPP (Fig. 2b), as in a recent study where CLM4.5 significantly underestimated GPP at a coniferous forest in northeastern United States (Duarte et al., 2017). GPP affects the substrate supply for SR, as evidenced by the close relationship between changes in SR and GPP (Fig. S1), which is consistent with experimental evidence showing GPP can directly affect the magnitude of root respiration (Craine et al., 1999; Högberg et al., 2001; Wan and Luo, 2003; Verburg et al., 2004; Gu et al., 2008). Second, the changed soil moisture scheme increased the moisture modifier (ξ_W) on heterotrophic respiration during the peak-growing season, and decreased it during the non-growing season (Fig. S2), which is consistent with the trend of changes in SWP (Fig. 3). In addition, the changed soil moisture scheme also increased the simulated SOC stock, the substrate for heterotrophic respiration (Fig. S3). These changes together resulted in the improvement of simulated SR.”*

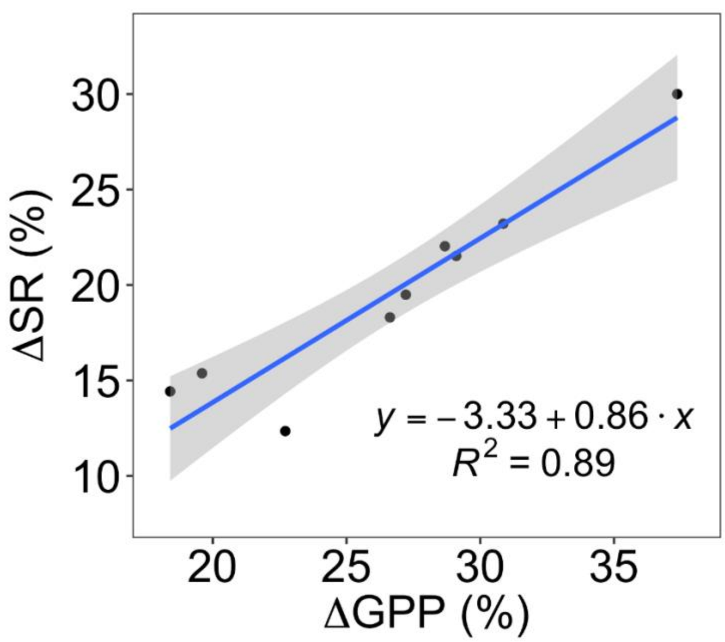

Figure S1: Relationship between changes in simulated annual soil respiration (ΔSR) and gross primary production (ΔGPP) induced by improvement of soil water potential using the Hanson model.

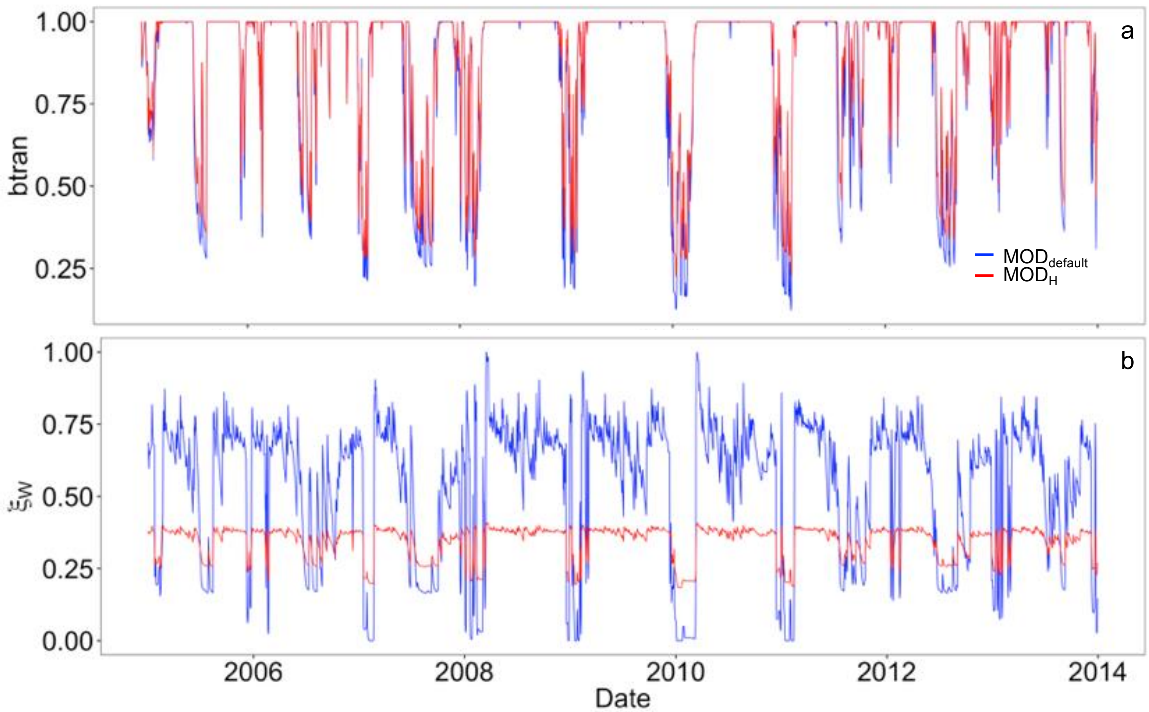

Figure S2 Impact of the changed SWP on the moisture modifiers of GPP (btran, a) and heterotrophic respiration (ξw, b). $MOD_{default}$: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement using the Hanson model.

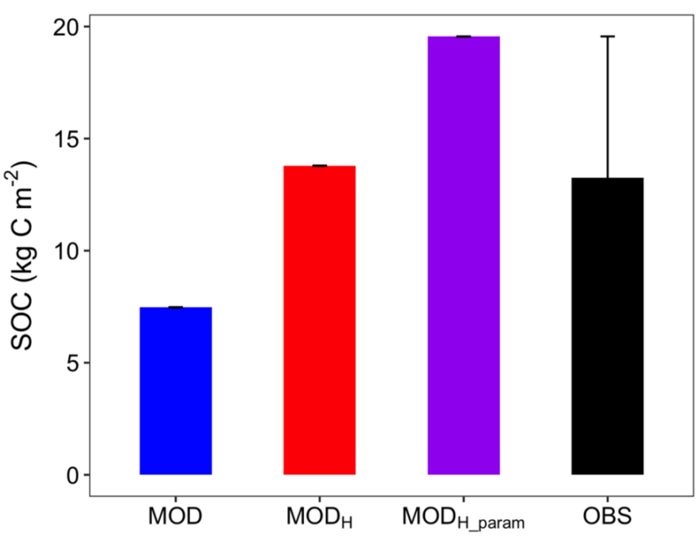

Figure S3 Comparison of the observed and modelled soil organic carbon (SOC) stocks. OBS: observation; MOD: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement using the Hanson model; MOD_{H_param}: model output after soil water potential improvement using the Hanson model and parameter adjustments.

Major concerns
I appreciate the effort used to explore alternative formulations for SWP in the model (Fig. 1, Table 1). Two questions come to mind. First, is it worth doing a more thorough model selection process like AIC or BIC that penalizes more complex models for their additional parameters instead of just showing RMSE. Second, as E3SM is intended to be run in global simulations, I wonder what effect alternative formulations for SWP have on water and energy fluxes from the model in site level, and ultimately global, simulations? The GPP results (Fig. 2) are a good start for this, but presumably these changes really modify ET fluxes (and runoff). It seems documenting these changes are likely important (if only in SI)?

Response: The reviewer provided valuable comments in terms of the model selection and the effect of the alternative formulations for SWP on water and energy fluxes. In the revised manuscript, we added Akaike Information Criterion (AIC), in addition to root-mean-square-error (RMSE), for the model selection. Both AIC and RMSE indicated that the Hanson model was the best in simulating the SWP-VWC relationship (i.e., smallest AIC and RMSE values; revised Table 1 and also see below).

Table 1. Root-mean-square-error (RMSE) and Akaike Information Criterion (AIC) of different models in simulating the SWP-VWC relationship for the soil in the MOFLUX site at two depths: 0 to 30 cm and below 30 cm.

	< 30 cm		> 30 cm	
Model	RMSE	AIC	RMSE	AIC
Clapp & Hornberger (default ELMv0)	4.25	157.82	1.33	18.51
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van Genuchten	0.50	-65.53	0.36	-36.61

In addition, we analyzed changes in simulated evapotranspiration (ET) and runoff as suggested. We plotted the mean annual cycle (± 1 sigma) of both ET and runoff (Fig. S6 and also see below). The change in soil moisture scheme using the Hanson model and parameter adjustments slightly increased ET and decreased runoff. Despite these slight changes, the model-simulated ET generally fell within the observed range, with or without changes in soil water scheme and parameters.

In the revised manuscript, we added a paragraph in the Results section to describe the changes in ET, runoff and other variables (page 10, lines 12 – 17):

"In addition, we analyzed changes in simulated evapotranspiration (ET), runoff, photosynthesis, net primary production, C allocations to fine roots, leaf and woody tissue in response to the changes in the soil water scheme and parameters (Fig. S6, S7). The change in soil moisture scheme and parameter adjustments slightly increased ET and decreased runoff.

Despite these slight changes, the model simulated ET generally fell within the observed range, with or without changes in soil water scheme and parameters (Fig. S6).”

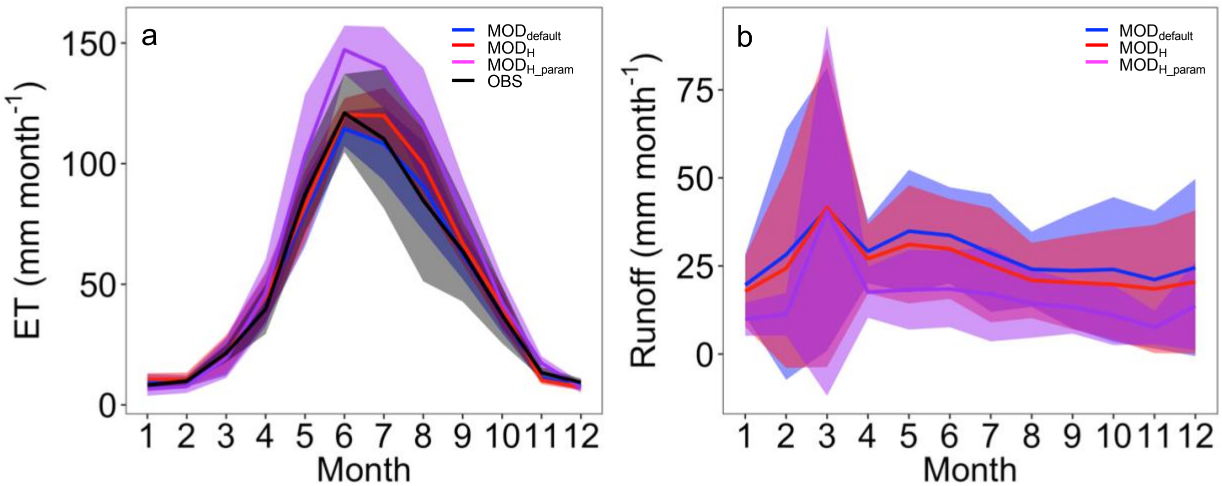

Figure S6 Modelled evapotranspiration (ET) and runoff in response to the improved SWP and parameter adjustments. OBS: observation; $MOD_{default}$: model output before soil water potential improvement; MOD_{H}: model output after soil water potential improvement using the Hanson model; MOD_{H_param}: model output after soil water potential improvement using the Hanson model and parameter adjustments.

If Hanson or van Genuchten formulations are ‘better’ fits to the observations, why aren’t they used for GPP simulations in Fig. 2? What’s the purpose of exploring alternative SWP schemes, if they don’t follow through the C cycle simulations in the model? Reading the text on the bottom of page 7, however, maybe (MODswp) is using the Hanson scheme? If so, does the calibrated Clapp & Hornberger approach provide similar improvement by removing the high bias in the default configuration (Fig. 3). Please clarify in the text and figure captions what’s being shown and why none of the models adequately capture the effect of the 2012 drought.

Response: We apologize for the unclear description in the manuscript. The Hanson model was used through the carbon cycle simulations in the model. As shown in Fig. S2, the changed soil water scheme had impacts on both the moisture modifiers of GPP and heterotrophic respiration. We have revised the text and figure captions to make it clearer.

In response to the question *“does the calibrated Clapp & Hornberger approach provide similar improvement by removing the high bias in the default configuration”*, we conducted an additional analysis as described in the response to the first comment above. We compared the simulated gross primary production (GPP) and soil respiration (SR) when using the Hanson model and the calibrated Clapp & Hornberger model. Generally, both the Hanson model and the calibrated Clapp & Hornberger model improved the simulation of GPP and SR in the ELMv0, in comparison with the default run (Fig. S8 and also see below). The ELMv0 with the Hanson model consistently produced higher GPP and SR than that with the calibrated Clapp & Hornberger model. In comparison with the observations, the modelled SR generally fell within the 1 sigma range of observations, for both the Hanson model and the calibrated Clapp & Hornberger model. However, the modelled GPP with the calibrated Clapp & Hornberger model was significantly lower than the observations. Given the order of the goodness-of-fit of the soil water SWP-VWC relationship was default Clapp & Hornberger model < calibrated Clapp & Hornberger model < Hanson model (revised Table 1 and also see below), these new results further support our conclusion that better representations of SWP can improve the simulations of carbon processes (i.e., GPP and SR here).

In the revised manuscript, we added a new supplementary figure (i.e., Fig. S8) and a paragraph in the text to compare simulations with the Hanson model and the calibrated Clapp & Hornberger model (page 12, lines 14 – 24):

"Moreover, we also explored whether the calibrated Clapp & Hornberger model can lead to similar improvements with the Hanson model (Fig. S8). Generally, both the Hanson model and the calibrated Clapp & Hornberger model improved the simulation of GPP and SR in the ELM, in comparison with the default run (Fig. S8). The ELMv0 with the Hanson model consistently produced higher GPP and SR than that with the calibrated Clapp & Hornberger model. In comparison with the observations, the modelled SR generally fell within the 1 sigma (i.e., standard deviation) range of observations, by using both the Hanson model and the calibrated Clapp & Hornberger model. However, the modelled GPP with the calibrated Clapp & Hornberger model was still lower than the observations. Given the order of the goodness-of-fit of the SWP-VWC relationship was default Clapp & Hornberger model < calibrated Clapp & Hornberger model < calibrated Hanson model (Table 1), these results further support the conclusion that better representations of SWP can improve the simulations of carbon processes. Therefore, throughout the remainder of this manuscript, we used the Hanson model to represent the SWP-VWC relationship."

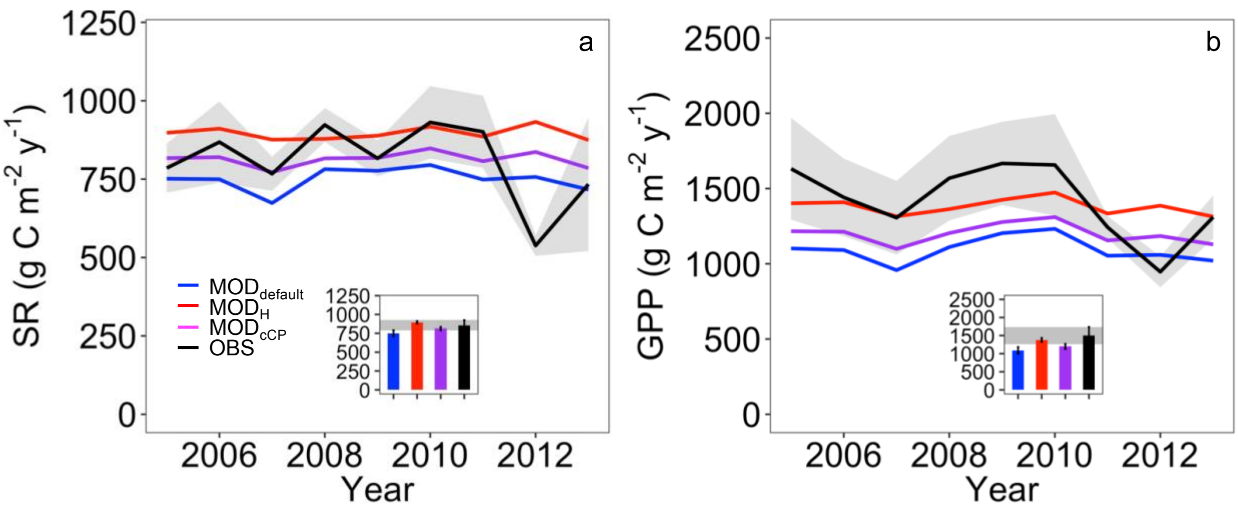

Figure S8: Annual soil respiration (SR) and gross primary production (GPP). Blue lines are the ELMv0 simulations with default parameters ($MOD_{default}$), red lines with the soil water potential improved using the calibrated Clapp & Hornberger model (MOD_{cCP}), and purple lines with the soil water potential improved using the Hanson model (MOD_H). Black lines and grey area are the observed (OBS) mean and 1 sigma range, which were calculated from eight field replications for SR, and from three different net ecosystem exchange partitioning methods for GPP. The inserted bar plots are mean annual average ± 1 sigma across 2005-2011.

In response to the question "*why none of the models adequately capture the effect of the 2012 drought*", we revised Section 4.2 to include more discussion. Failing capturing the effect of the 2012 drought, as well as the underestimated seasonal and interannual variabilities of GPP and SR (Fig. 2, 4), indicate that the current model structure is not sensitive enough to environmental changes. Potential reasons include lacking representations of microbial organisms, macroinvertebrate and other forest floor and soil fauna and root exudates. We discussed in detail in Section 4.2 as:

"Although the simulation of the SWP using the Hanson model improved the representation of both annual SR and GPP, the model continued to overestimate SR during the non-growing season (Figs. 4), resulting in significant overestimations of the annual SR fluxes (Fig. S5). In addition, no matter which SWP simulations were used, the ELMv0 had smaller interannual variability than the observations (Fig. 2). Specifically, the model was not able to capture the steep decreases in GPP and SR in the extreme drought year (i.e., 2012). These results indicate that the current model structure is not sensitive enough to environmental changes. A few potential reasons may contribute to the underestimated seasonal and interannual variability. In the ELMv0, heterotrophic respiration contributed a majority proportion (i.e., over 85%) to total SR during non-growing seasons (Fig. 5), suggesting that the overestimation of SR during these seasons was primarily due to the biased heterotrophic respiration simulation. A potential reason for the biased simulation of heterotrophic respiration may be related to the temperature sensitivity (Q_{10}). Theoretically, a higher Q_{10} can result in greater seasonal variability of SR (Fig. S9). Compared to relatively small Q_{10} values, a larger Q_{10} can lead to lower heterotrophic respiration when temperature is below the reference temperature, and greater heterotrophic respiration when temperature is above the reference (Fig. S9). In the ELMv0, the reference temperature is 25 ºC and the Q_{10} of heterotrophic respiration is 1.5 (Oleson et al., 2013). A previous study derived a much greater Q_{10} value (i.e., 2.8) when the parameters were calibrated with data from another temperate forest (Mao et al., 2016). We hypothesized that the Q_{10} value of 1.5 may be too small for the MOFLUX site. We arbitrarily increased Q_{10} from 1.5 to 2.5, but there were minimal effects on the SR simulation (Fig. S10). This indicates that modifying the temperature sensitivity of heterotrophic respiration may not improve the modelled representation of seasonality of SR in the ELMv0.

Another potential reason for the biased simulation of heterotrophic respiration may be that the seasonality of microbial organisms was not adequately represented in the model. Like most ESMs, the ELMv0 represents soil C dynamics using linear differential equations and assumes that SR is a substrate-limited process in the model. However, producers of CO_2 in soils, microbial organisms, have a significant seasonal cycle (Lennon and Jones, 2011). These organisms usually have very high biomass and activity during the peak growing season, with favorable conditions of temperature, moisture and substrate supply, and tend to be dormant under stressful conditions in non-growing seasons (Lennon and Jones, 2011; Stolpovsky et al., 2011; Wang et al., 2014; Wang et al., 2015). The seasonality of microbial biomass and activity, in addition to that of GPP and ST, may contribute to the seasonal variability of SR.

Additionally, another reason may be related to the model lacking representation of macroinvertebrate and other forest floor and soil fauna. There is a high density of earthworms at the MOFLUX site (Wenk et al., 2016). Earthworms can shred and redistribute soil C and change soil aggregation structure, which may alter soil C dynamics and CO_2 efflux to the atmosphere

(Verhoef and Brussaard, 1990; Brussaard et al., 2007; Coleman, 2008). Like microbial organisms, earthworms usually have a significant seasonal cycle, showing high biomass and high activity during peak growing seasons and tending to be dormant during non-growing seasons (Wenk et al., 2016). However, a recent review suggests that current experimental evidence and conceptual understanding remains insufficient to support the development of explicit representation of fauna in ESMs (Grandy et al., 2016). Therefore, data collection focused on seasonal variations in fauna and microbial biomass and activity might enable further improvements in the representation of seasonal variation in SR.

Our analyses also showed that the modelled SR was not able to reach the observed peak in many years during the peak growing season even when the modelled GPP exceeded the observation. In addition, the parameter modification increased GPP during both peak and non-growing seasons, resulting in an even greater overestimation of SR during non- growing seasons. These results suggest that simply increasing GPP may not be adequate to increase the seasonal variability of the simulated SR. A potential reason may be that the current model does not include root exudates. Root exudates are labile C substrates that are important for SR (Kelting et al., 1998; Kuzyakov, 2002; Sun et al., 2017). The root exudate rate is primarily dependent on root growth, showing a seasonal cycle in temperate forests (Kelting et al., 1998; Kuzyakov, 2002). Thus, including root exudates in the model may further increase the model simulated SR during the peak growing season without needing to increase GPP."

Minor concerns

Section 2.3 This is really a broader comment on how author groups working with E3SM intend to articulate the version of the model on which they are working, esp. for readers less familiar with nuances of CLM4.5 development branches and subsequent ELM developments. For example, how is this code different from other publications (e.g. Brunke et al. 2016; Riley 2018)?

Section 2.3. Please justify the decision to use the CLM-CN decomposition module for a paper focused on soil respiration when Bonan and others (2013) clearly demonstrated shortcomings of this model version? It seems like the wrong tool for this job?

Section 2.3. This is also a little confusing, as the opening line of the section states the soil biogeochemistry is vertically resolved, but to my knowledge CLM-CN does not apply vertically resolved soil BGC? Please clarify

Response: We appreciate the detailed comments on the model version. We used the ELM version 0 (ELMv0), which is equivalent to the Community Land Model version 4.5 (CLM 4.5). In the ELMv0, the soil biogeochemistry can be simulated with one-layer or multi-layer converging trophic cascade (CTC, i.e., CLM-CN) decomposition model. We used the vertically-resolved CTC decomposition in this study. Variable thickness of the soil profile in Brunke et al. (2016) and lateral energy and hydrological exchanges in Bisht et al. (2018) (which may be the paper (Riley, 2018) the reviewer referred to) were not in the ELMv0.

In response to the comment "*It seems like the wrong tool for this job*", we used the ELMv0, which is structurally equivalent to the CLM 4.5. Recently, the E3SM council completed a comprehensive study of the soil biogeochemistry module by benchmarking different approaches with global (e.g., ILAMB) and Ameriflux datasets. Due to satisfactory overall performance of the CTC approach (i.e., CLM-CN), the council recommended the CTC approach as the default and baseline soil decomposition pathway in future ELM development. Therefore, we decided to use the CTC decomposition pathway in each soil layer for our study.

In the revised manuscript, we revised this section as (page 3, lines 28 – 31):

"The ELMv0 used in this study is structurally equivalent to the Community Land Model 4.5 (CLM 4.5), which includes coupled carbon and nitrogen cycles (Oleson et al., 2013). In ELMv0, the soil biogeochemistry can be simulated with one-layer or multi-layer converging trophic cascade (CTC, i.e., CLM-CN) decomposition model. We used the vertically-resolved CTC decomposition in this study."

Page 4, Line 20. Single point runs (especially with CLM) forced with flux tower measurements have a long history that should be acknowledged here.

Response: We add a sentence to acknowledge the long history of single point runs (page 4, lines 22 – 24):

"Single-point runs forced with site-level measurements have a long history to evaluate model representations of phenology, NPP, transpiration, LAI, water use efficiency, and nitrogen use efficiency (Richardson et al., 2012; De Kauwe et al., 2013; Walker et al., 2014; Zaehle et al., 2014; Mao et al., 2016; Duarte et al., 2017; Montané et al., 2017)."

Page 7, Line 7. What changes were made to the Clapp and Hornberger parameterization, there are lots of hard coded parameters in eq. 11-13.

Response: For the calibration of the Clapp & Hornberger model, instead of using the hard-coded parameters in Eq. 11-13, we calibrated the three parameters (i.e., Ψ_m, θ_s and Ψ_s) in the Clapp & Hornberger model (Eq. 10). We added the sentence in the **Materials and Methods** section (page 6, lines 5 – 7):

"For the calibration of the Clapp & Hornberger model, instead of using the hard-coded (default) parameters in Eq. 11-13, we calibrated the three parameters (i.e., Ψ_m, θ_s and Ψ_s) in the Clapp & Hornberger model (Eq. 10)."

Fig 2. Why are observations shown with a black line and purple bar (inset)? Consistency within and among figures will help readers understand display items more easily? Similarly, using the same color for line of the default model and modified model in Figs. 1 and 2 would be helpful One strength of using flux tower data in single point simulations seems to be examining the seasonal cycle of carbon and energy fluxes. This is somewhat lost in Fig. 6, and I wonder if the display item would be more powerful if simulations are results were averaged over the whole observation record (e.g. just show 1 year instead of 9, as the interannual variability isn't that obvious (and already shown in Fig. 2)

Response: We really appreciate the great suggestion on the figure display. In the revised manuscript, we used consistent colors. In addition, we re-plotted Fig. 6 (revised Fig. 4) as the mean annual cycle (with 1 sigma) as suggested here and in a few other comments.

Fig 4 is never really discussed and doesn't add much to the paper in my estimation. Can it be removed from the text? More, it follows that that changes in productivity would have a linear effect on soil C stocks and therefore respiration rates in a first order model like CLM-cn (Todd-Brown refs from the text), so the relationship shown here isn't really surprising.

Response: We moved Fig. 4 to Fig. S1 as discussed above.

Out of curiosity, how do simulated soil (or vegetation) C stocks compare with observed stocks at the site? The focus on fluxes is fine, but given that fluxes are linear related with stocks, do suggested modifications to the model improve estimates of fluxes AND stocks for the site?

Response: This is really an insightful comment. We analyzed the modelled soil organic carbon (SOC) stocks in the revised manuscript (Fig. S3 and also see below). Although the improved SWP simulations increased SOC stocks, the model simulated SOC with different soil water schemes and parameters generally fell within the wide range of observations.

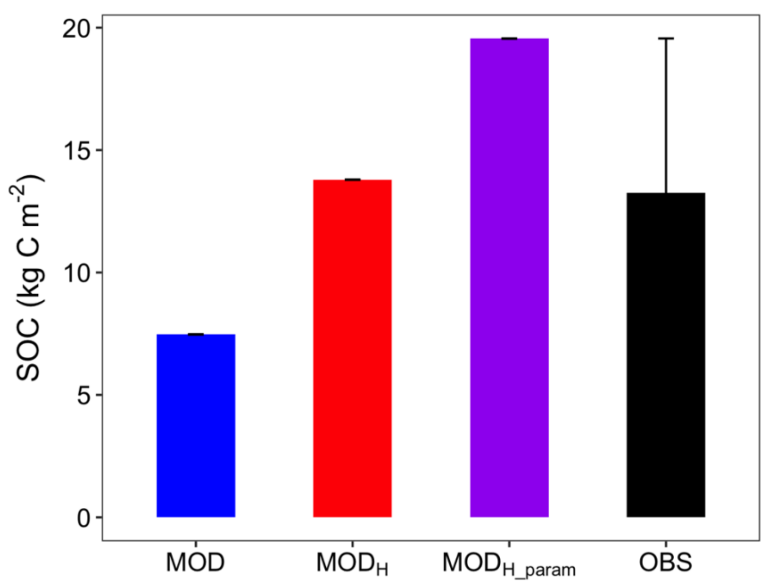

Figure S3 Comparison of the observed and modelled soil organic carbon (SOC) stocks. OBS: observation; MOD: model output before soil water potential improvement; MOD$_H$: model output after soil water potential improvement using the calibrated Hanson model; MOD$_{H_param}$: model output after soil water potential improvement using the calibrated Hanson model and parameter adjustments.

In the revision, we added the description of the result on page 8, lines 4 – 6 as:

"While SOC when simulated by the model with different soil water schemes generally fell within the wide range of observations, the improved SWP simulations using the Hanson model increased SOC stocks (Fig. S3)."

Seasonal biases in SR and GPP fluxes look pretty bad with default and 'swp' versions of the model (Fig. 5). The parametric changes in Table 2 seem to address some of these seasonal biases (Fig. 6), but it seems like showing the scatter plots on Fig. 5 (maybe with a 3rd color) would be helpful? Along these lines, should both Figs. 5 and 6 show the same 3 simulation ('default', 'swp', and 'swp_param')? Showing the mean annual cycle (+/- 1 sigma on the observations) for all panels in Fig. 6 would help to make this figure easier to digest.

Response: In the revision, we re-plotted Fig. 6 (revised Fig. 4 and also see below) as the mean annual cycle (with 1 sigma) as suggested. We included all 'default', 'H', 'H_param', and 'obs' in the figure. The revised figure can clearly show the seasonal biases in SR and GPP fluxes. Thus, the original Fig. 5 was duplicated by this presentation, so we deleted Fig. 5 in the revised manuscript. Because we moved the original Fig. 4 to Fig. S1, the original Fig. 6 is Fig. 4 in the revised manuscript.

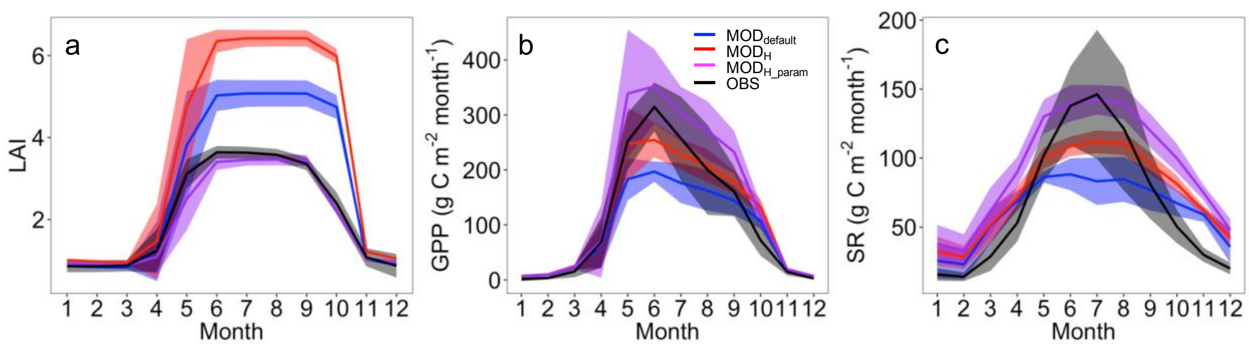

Figure 4 The annual mean cycles of leaf area index (LAI), gross primary production (GPP) and soil respiration (SR). OBS: observation; $MOD_{default}$: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement by the Hanson model; MOD_{H_param}: model output after soil water potential improvement by the Hanson model and parameter adjustments.

SLA is something that's measured, maybe not at the site for similar trees to the ones at the site? Is building 3x thicker leaves (Table 2), a reasonable assumption? Similarly, if the authors need to decrease LAI while increasing GPP, flnr necessarily has to increase in the model, but is the 20% increase here supported by databases like TRY, or are these parameter changes just illustrating big nobs in the model that are poorly constrained by observaions?

Response: We appreciate the detailed suggestion on parameter values. Unfortunately, SLA was not measured at the site. The parameter adjustments were based on a surrogate based global optimization using measurements of C and energy fluxes at the site (Lu et al., 2018). The TRY database showed that the SLA for broadleaved deciduous forest ranges from < 0.005 to > 0.05 $m^2 g^{-1}$ C, with mean values of 0.015 $m^2 g^{-1}$ C (Kattge et al., 2011). Thus, the adjustment of the parameter *slatop* fell within the range of observations.

Page 10, line 12 please report statistics to support claims being made. Visually, the red line looks closer to the observations than the blue one (Fig. 6b,c). How do the annual totals look?

As with comment above, how do changes in annual fluxes or total stocks compare with observations following parametric changes suggested in Table 2?

Response: We replotted Fig. 6 (Fig. 4 in the revision) to show the annual cycle ± 1 sigma considering all 9 years of data. With the revised figure, we can methodically step through the changes. Results showed that both the default and improved SWP using the Hanson model overestimated the maximum LAI (Fig. 4a). The parameter changes significantly reduced the maximum LAI to better match the observations (Fig. 4a). The parameter changes further increased the simulated GPP and SR during the peak growing season, in addition to the improvement by the adjusted SWP (Fig. 4b, c). However, the ELMv0 still overestimated SR during the non-growing season.

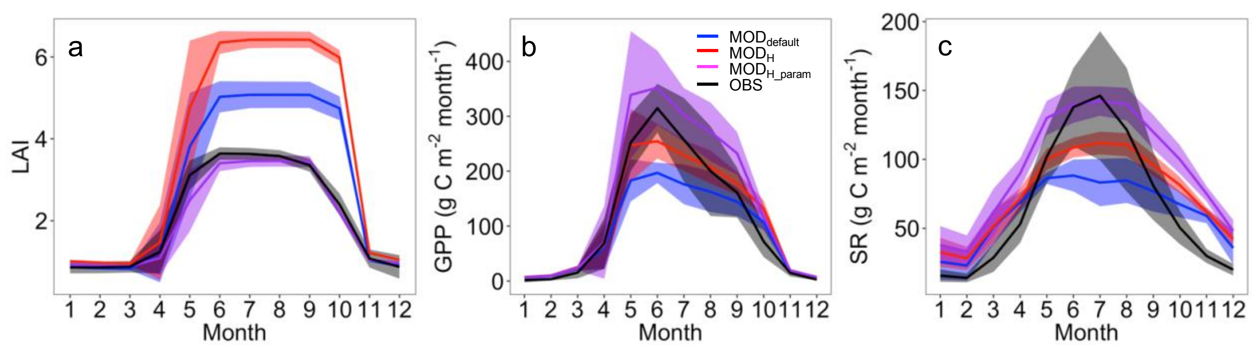

Figure 4 The annual mean cycles of leaf area index (LAI), gross primary production (GPP) and soil respiration (SR). OBS: observation; $MOD_{default}$: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement by the Hanson model; MOD_{H_param}: model output after soil water potential improvement by the Hanson model and parameter adjustments.

To answer the question "*how do the annual totals look*", we analyzed the mean annual fluxes of GPP and SR (Fig. S5 and also see below) and SOC stocks (Fig. S3 and also see below). After the parameter adjustments, GPP was still within the observed ranges, while SR was significantly overestimated due to the overestimation of SR during the non-growing season. In Section 4.2, we discussed the potential reasons, including Q_{10} and representations of microbial organisms, macroinvertebrate and other forest floor and soil fauna.

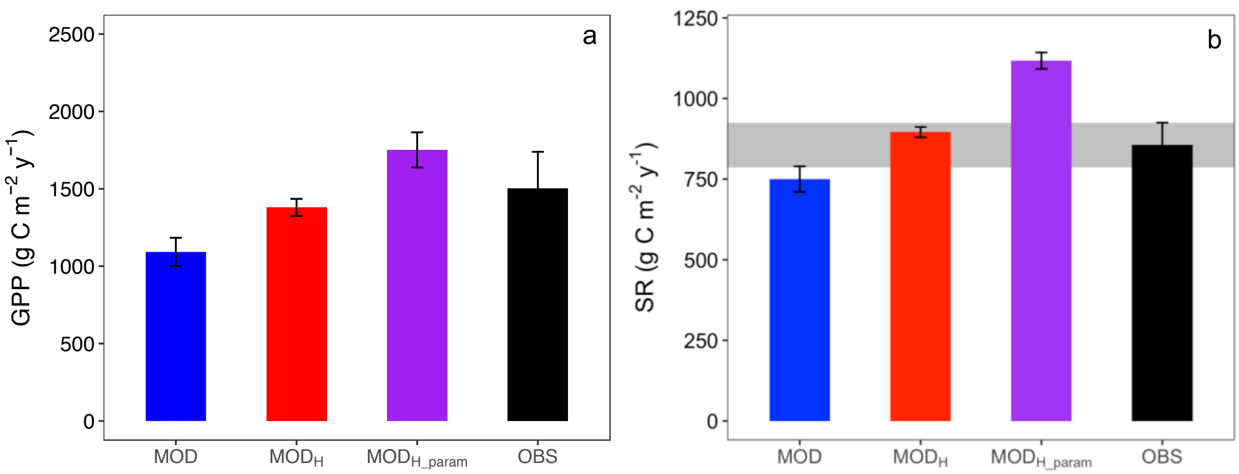

Figure S5 Comparison of the observed and modelled gross primary production (GPP) and soil respiration (SR). OBS: observation; MOD: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement using the calibrated Hanson model; MOD_{H_param}: model output after soil water potential improvement using the calibrated Hanson model and parameter adjustments.

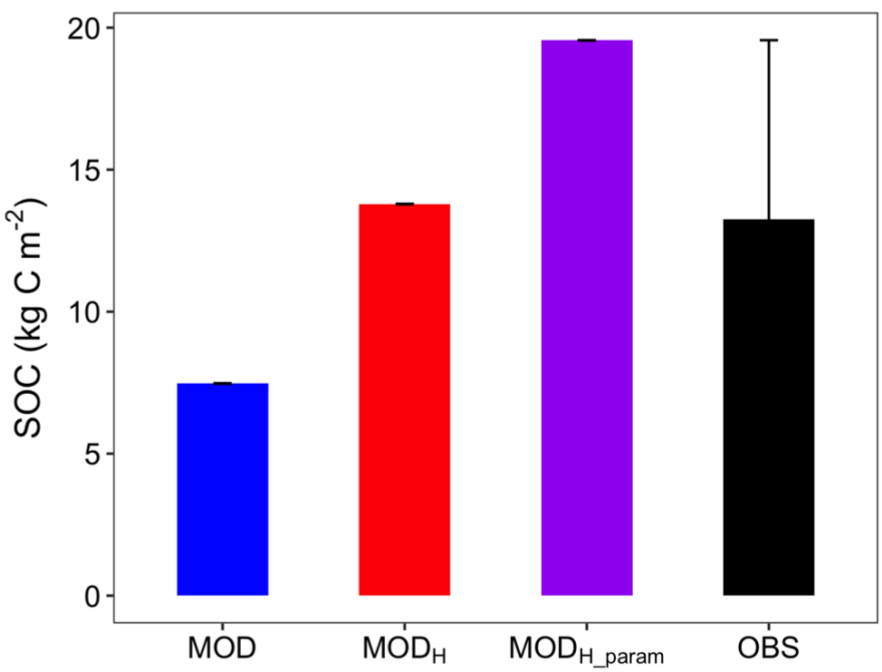

Figure S3 Comparison of the observed and modelled soil organic carbon (SOC) stocks. OBS: observation; MOD: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement using the calibrated Hanson model; MOD_{H_param}: model output after soil water potential improvement using the calibrated Hanson model and parameter adjustments.

In the revision, we added the new results (page 10, lines 6 – 12):

"Results showed that the ELMv0 with both the default and improved SWP by the Hanson model overestimated the maximum LAI (Fig. 4a). The adjustment of the aforementioned five parameters (Table 2) significantly reduced the LAI to within a more reasonable range (Fig. 4a). The parameter changes further increased the simulated GPP and SR during the peak growing season, in addition to the improvement by the adjusted SWP (Fig. 4b, c). However, all modifications of the ELMv0 still overestimated SR during the non-growing season, resulting in significant overestimation of annual SR fluxes (Fig. S5a). After the parameter adjustments, the annual GPP flux was still within the observed range (Fig. S5b)."

We also discussed the potential reasons in Section 4.2:

"Although the simulation of the SWP using the Hanson model improved the representation of both annual SR and GPP, the model continued to overestimate SR during the non-growing season (Figs. 4), resulting in significant overestimations of the annual SR fluxes (Fig. S5). In addition, no matter which SWP simulations were used, the ELMv0 had smaller interannual variability than the observations (Fig. 2). Specifically, the model was not able to capture the steep decreases in GPP and SR in the extreme drought year (i.e., 2012). These results indicate that the current model structure is not sensitive enough to environmental changes. A few potential reasons may contribute to the underestimated seasonal and interannual variability. In the ELMv0, heterotrophic respiration contributed a majority proportion (i.e., over 85%) to total SR during non-growing seasons (Fig. 5), suggesting that the overestimation of SR during these seasons was primarily due to the biased heterotrophic respiration simulation. A potential reason for the biased simulation of heterotrophic respiration may be related to the temperature sensitivity (Q_{10}). Theoretically, a higher Q_{10} can result in greater seasonal variability of SR (Fig. S9). Compared to relatively small Q_{10} values, a larger Q_{10} can lead to lower heterotrophic respiration when temperature is below the reference temperature, and greater heterotrophic respiration when temperature is above the reference (Fig. S9). In the ELMv0, the reference temperature is 25 ºC and the Q_{10} of heterotrophic respiration is 1.5 (Oleson et al., 2013). A previous study derived a much greater Q_{10} value (i.e., 2.8) when the parameters were calibrated with data from another temperate forest (Mao et al., 2016). We hypothesized that the Q_{10} value of 1.5 may be too small for the MOFLUX site. We arbitrarily increased Q_{10} from 1.5 to 2.5, but there were minimal effects on the SR simulation (Fig. S10). This indicates that modifying the temperature sensitivity of heterotrophic respiration may not improve the modelled representation of seasonality of SR in the ELMv0.

Another potential reason for the biased simulation of heterotrophic respiration may be that the seasonality of microbial organisms was not adequately represented in the model. Like most ESMs, the ELMv0 represents soil C dynamics using linear differential equations and assumes that SR is a substrate-limited process in the model. However, producers of CO_2 in soils, microbial organisms, have a significant seasonal cycle (Lennon and Jones, 2011). These organisms usually have very high biomass and activity during the peak growing season, with favorable conditions of temperature, moisture and substrate supply, and tend to be dormant under stressful conditions in non-growing seasons (Lennon and Jones, 2011; Stolpovsky et al., 2011; Wang et al., 2014; Wang et al., 2015). The seasonality of microbial biomass and activity, in addition to that of GPP and ST, may contribute to the seasonal variability of SR.

Additionally, another reason may be related to the model lacking representation of macroinvertebrate and other forest floor and soil fauna. There is a high density of earthworms at the MOFLUX site (Wenk et al., 2016). Earthworms can shred and redistribute soil C and change soil aggregation structure, which may alter soil C dynamics and CO_2 efflux to the atmosphere (Verhoef and Brussaard, 1990; Brussaard et al., 2007; Coleman, 2008). Like microbial organisms, earthworms usually have a significant seasonal cycle, showing high biomass and high activity during peak growing seasons and tending to be dormant during non-growing seasons (Wenk et al., 2016). However, a recent review suggests that current experimental evidence and conceptual understanding remains insufficient to support the development of explicit representation of fauna in ESMs (Grandy et al., 2016). Therefore, data collection focused on seasonal variations in fauna and microbial biomass and activity might enable further improvements in the representation of seasonal variation in SR.

Our analyses also showed that the modelled SR was not able to reach the observed peak in many years during the peak growing season even when the modelled GPP exceeded the observation. In addition, the parameter modification increased GPP during both peak and non-growing seasons, resulting in an even greater overestimation of SR during non- growing seasons. These results suggest that simply increasing GPP may not be adequate to increase the seasonal variability of the simulated SR. A potential reason may be that the current model does not include root exudates. Root exudates are labile C substrates that are important for SR (Kelting et al., 1998; Kuzyakov, 2002; Sun et al., 2017). The root exudate rate is primarily dependent on root growth, showing a seasonal cycle in temperate forests (Kelting et al., 1998; Kuzyakov, 2002). Thus, including root exudates in the model may further increase the model simulated SR during the peak growing season without needing to increase GPP."

Page 12, line 4. This doesn't seem like a fair statement or comparison, as results from the tuned Clapp & Hornberger scheme are never presented.

Response: In the revision, we compared the ELMv0 simulations with the Hanson model and the calibrated Clapp & Hornberger scheme as described above. The performance of the Hanson model was better than the calibrated Clapp & Hornberger model. Thus, we used the Hanson model to improve the SWP simulations.

Page 12, line 10, given the dominance of Rh in contributions to soil respiration (Fig 7). I'd suspect that changes in SR have more to do with larger SOM stocks than they do links between substrate supply through GPP, as suggested here, but no data are presented along these lines?

Response: As described above, the improved SR was a joint result of changes in GPP, SOC stocks and the moisture modifier of heterotrophic respiration. We revised this part (page 11, lines 4 – 14) as:

"The improvements in model fits were due to changes in GPP, SOC stocks, and the moisture modifier on heterotrophic respiration (Figs. S1 – S3). First, the default ELMv0 underestimated GPP (Fig. 2b), as in a recent study where CLM4.5 significantly underestimated GPP at a coniferous forest in northeastern United States (Duarte et al., 2017). GPP affects the substrate supply for SR, as evidenced by the close relationship between changes in SR and GPP (Fig. S1), which is consistent with experimental evidence showing GPP can directly affect the magnitude of

root respiration (Craine et al., 1999; Högberg et al., 2001; Wan and Luo, 2003; Verburg et al., 2004; Gu et al., 2008). Second, the changed soil moisture scheme increased the moisture modifier (ξ_W) on heterotrophic respiration during the peak-growing season, and decreased it during the non-growing season (Fig. S2), which is consistent with the trend of changes in SWP (Fig. 3). In addition, the changed soil moisture scheme also increased the simulated SOC stock, the substrate for heterotrophic respiration (Fig. S3). These changes together resulted in the improvement of simulated SR."

Page 12, line 20. This statement may be true, but it's not clear that changes to VMC proposed here had much of an effect on the Rh component of the model. To show this, it seems like showing the soil moisture effect (w_scalar) on soil decomposition rates from different configurations of the model would be needed. Otherwise, I'd suspect that improvement to SR (Fig 2, 5) are predominantly driven by larger soil C stocks (via higher GPP), but not from direct improvement in the SWC on soil biogeochemistry, as suggested in the Powell paper referenced.

Response: The soil moisture modifier (w_scalar, which is ξ_W in Eq. 9) of heterotrophic respiration was shown in Fig. S2 (and also see below) in the revision. In addition, the SOC stocks under different schemes were shown in Fig. S3. As discussed above, the improvement of SR was a joint result of changes in GPP, SOC stocks and the moisture modifier.

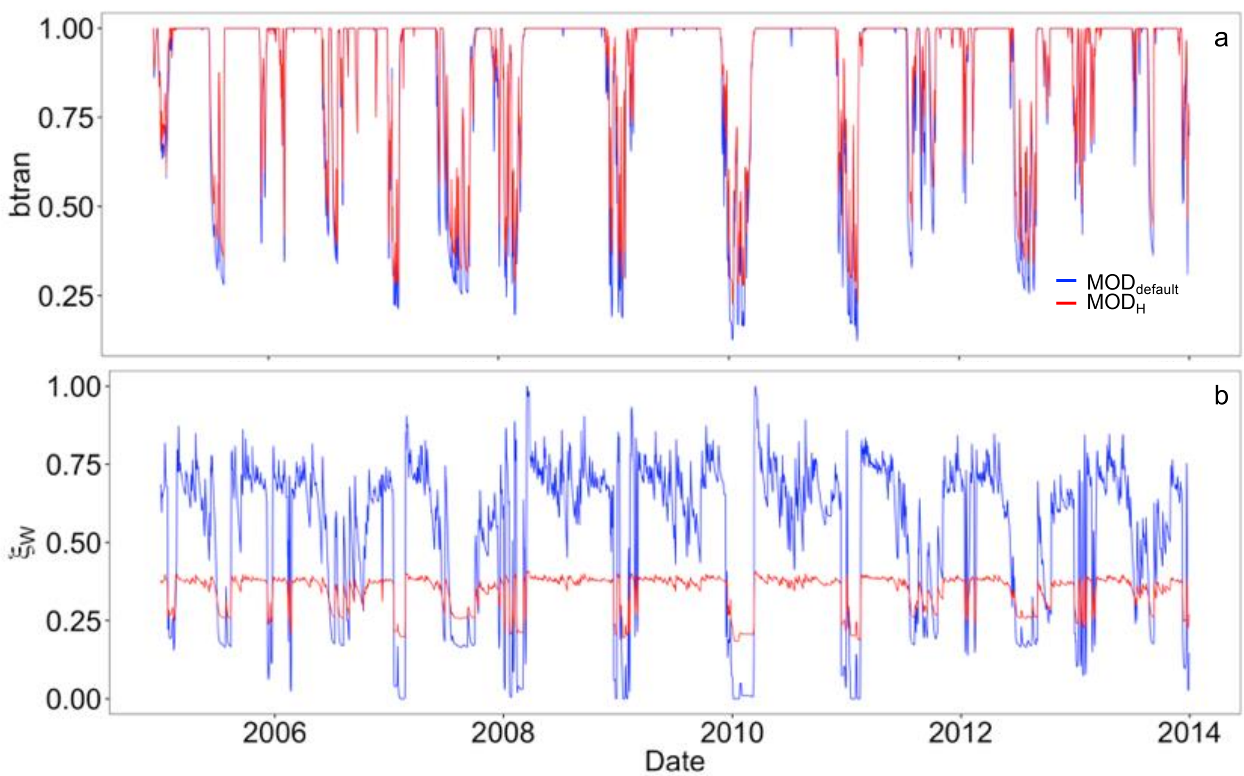

Figure S2 Impact of the changed SWP on the moisture modifiers of GPP (btran, a) and heterotrophic respiration (ξ_W, b). $MOD_{default}$: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement using the Hanson model.

Page 12, line 20 what is SWP-VMC, should be VWC?

Response: Yes and revised.

Page 13, line 2. Again this claim is poorly supported by the data presented. Yes, the tuned Clapp and Hornberger model is not the 'best' model in Table 1, but are results for GPP or SR markedly different than the Hansen results shown?

Response: Yes, the results for GPP and SR were markedly different when using the Hanson model and the calibrated Clapp & Hornberger model as discussed above. The ELMv0 with the Hanson model consistently produced higher GPP and SR than that with the calibrated Clapp & Hornberger model. In comparison with the observations, the modelled SR generally fell within the 1 sigma (i.e., standard deviation) range of observations, by using both the Hanson model and the calibrated Clapp & Hornberger model. However, the modelled GPP with the calibrated Clapp & Hornberger model was lower than the observations.

In response to the reviewer's concern, we deleted the sentence in the revision.

Page 14. The q10 analysis is nice, but I wonder if a more ecological explanation is relevant here- specifically highlighting the role of root exudates in supplying labile C substrates that are important for SR? The land model here doesn't consider these ecologically important C fluxes that likely have an important control over the seasonal dynamics of soil respiration and microbial biomass already discussed?

Response: The reviewer provided a great potential reasons for the modelled biases of SR. In the revision, we added the discussion of root exudates as (page 14, lines 12 – 20):

"Our analyses also showed that the modelled SR was not able to reach the observed peak in many years during the peak growing season, even when the modelled GPP exceeded the observation. In addition, the parameter modification increased GPP during both peak and non-growing seasons, resulting in an even greater overestimation of SR during non-growing seasons. These results suggest that simply increasing GPP may not be adequate to increase the seasonal variability of the simulated SR. A potential reason may be that the current model does not include root exudates. Root exudates are labile C substrates that are important for SR (Kelting et al., 1998; Kuzyakov, 2002; Sun et al., 2017). The root exudate rate is primarily dependent on root growth, showing a seasonal cycle in temperate forests (Kelting et al., 1998; Kuzyakov, 2002). Thus, including root exudates in the model may further increase the model simulated SR during the peak growing season without needing to increase GPP."

References: Bonan, et al (2013) Evaluating litter decomposition in earth system models with long-term litterbag experiments: an example using the Community Land Model version 4 (CLM4), Global Change Biology, 19, 957-974.

Brunke et al. 2016. "Implementing and Evaluating Variable Soil Thickness in the Community Land Model, Version 4.5 (CLM4.5)." Journal of Climate 29(9): 3441-3461, doi:10.1175/JCLI-D-15-0307.1.

Riley, W. 2018. "Impacts of Microtopographic Snow Redistribution and Lateral Sub- surface Processes on Hydrologic and Thermal States in an Arctic Polygonal Ground Ecosystem: A Case Study Using ELM-3D v1.0." Geoscientific Model Development 11(1): 61-76, doi:10.5194/gmd-11-61-2018.

Response: We appreciate the information!

Reviewer 2

This paper reports an effort of tuning an Earth system model, E3SM, to fit observed leaf area index (LAI), gross primary production (GPP, derived from eddy flux data), and soil respiration at a temperate deciduous forest site. The authors specifically tested different empirical relationships between volumetric water content (VWC) and soil water potential (SWP), and found tuning soil water potential improve the simulation of soil respiration. So, they concluded that "modelling soil respiration can be significantly improved by better model representations of the soil water retention curve." I agree with the authors that the well data-constrained model, Hanson model, increased the prediction of soil water potential, and may improve the simulation of GPP, which have been shown by the results (Figs. 3 and 7). But for the improvement of soil respiration, I think it's just a coincidence. From the Fig. 5a (page 9), we can see the new VMC-SWP relationship (i.e., Hanson model) increases soil respiration rate overall, but it does NOT change the pattern. This means the performance of soil respiration modeling is not improved. The authors also pointed out that the original model underestimates GPP and soil respiration (Line 13, page 7, and Fig. 2). So, the improvement of soil respiration prediction was not due to the improvement of SWP simulation, but because increases in GPP. The increases in GPP may increase carbon allocation to roots or total soil carbon, and therefore increase soil respiration. And, according to Fig. 7, the most possible reason for underestimating soil respiration is that the root respiration is not high enough in growing season, which also leads to the seasonal pattern that does not fit the observations because root respiration is usually high in growing season and very low in non-growing season.

Response: We greatly appreciate the valuable comment. The reviewer criticized that "*the improvement of soil respiration prediction was not due to the improvement of SWP simulation, but because increases in GPP*". A similar comment was raised by the first reviewer who commented that "*it's not clear if this is a direct effect of soil moisture on soil respiration*". We appreciate both the reviewers pointed the issue out. In response to the comments, we analyzed the changes in the soil moisture modifiers of GPP (btran) and heterotrophic respiration (ξ_W) and soil organic carbon (SOC) (Fig. S2-S3 and also see below), as suggested by the first reviewer. The improved soil water scheme using the Hanson model increased both *btran* and ξ_W during the peak growing season, and reduced ξ_W during the non-growing season (Fig. S2). While the model-simulated SOC with different soil water schemes generally fell within the wide range of observations, the improved SWP simulations increased SOC stocks (Fig. S3). These results, combining with previous results (revised Fig. S1), indicate that the improved annual fluxes of SR by SWP was a joint result of changes in GPP, SOC stocks and the moisture modifier on heterotrophic respiration.

In the revised manuscript, we added two new supplementary figures (Fig. S2, S3), moved Fig. 4 as Fig. S1, presented the results (page 8, lines 1 – 6) and discussed details (page 11, lines 3 – 14) in the text.

"The changes in annual SR and GPP (i.e., the differences between before and after the improved SWP simulation using the Hanson model) showed a linear relationship (Fig. S1). In addition, the improved soil water scheme using the Hanson model increased both the moisture modifiers of GPP and heterotrophic respiration (i.e., btran and ξ_W) during the peak growing season, and reduced ξ_W during the non-growing season (Fig. S2). While SOC when simulated by the model with different soil water schemes generally fell within the wide range of observations, the improved SWP simulations using the Hanson model increased SOC stocks (Fig. S3)."

"Constraining the SWP-VWC relationship with site-specific data and using the Hanson model instead of the ELMv0 default model (Fig. 1) significantly improved the model representation of SWP (Fig. 3) and annual SR (Fig. 2a). The improvements in model fits were due to changes in GPP, SOC stocks, and the moisture modifier on heterotrophic respiration (Figs. S1 – S3). First, the default ELMv0 underestimated GPP (Fig. 2b), as in a recent study where CLM4.5 significantly underestimated GPP at a coniferous forest in northeastern United States (Duarte et al., 2017). GPP affects the substrate supply for SR, as evidenced by the close relationship between changes in SR and GPP (Fig. S1), which is consistent with experimental evidence showing GPP can directly affect the magnitude of root respiration (Craine et al., 1999; Högberg et al., 2001; Wan and Luo, 2003; Verburg et al., 2004; Gu et al., 2008). Second, the changed soil moisture scheme increased the moisture modifier (ξ_W) on heterotrophic respiration during the peak-growing season, and decreased it during the non-growing season (Fig. S2), which is consistent with the trend of changes in SWP (Fig. 3). In addition, the changed soil moisture scheme also increased the simulated SOC stock, the substrate for heterotrophic respiration (Fig. S3). These changes together resulted in the improvement of simulated SR."

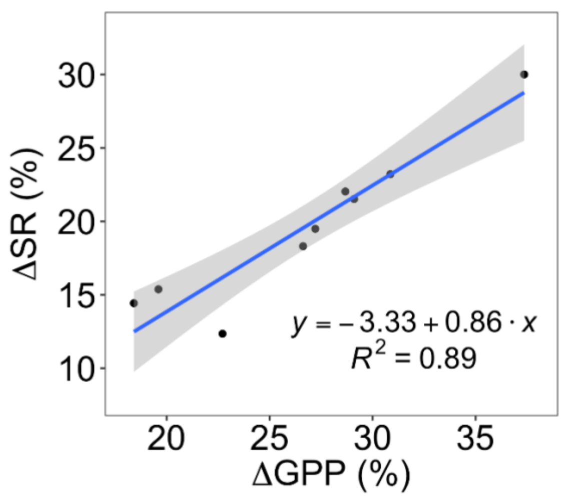

Figure S1: Relationship between changes in simulated annual soil respiration (ΔSR) and gross primary production (ΔGPP) induced by improvement of soil water potential using the Hanson model.

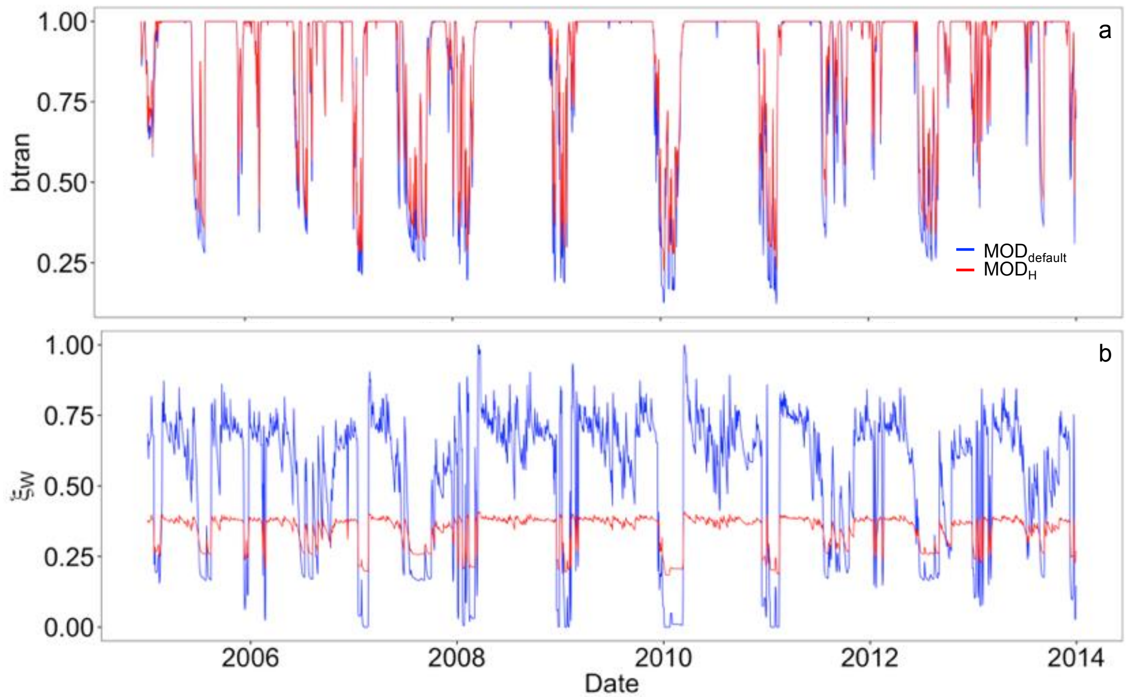

Figure S2 Impact of the changed SWP on the moisture modifiers of GPP (btran, a) and heterotrophic respiration (ξ_W, b). $MOD_{default}$: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement using the Hanson model.

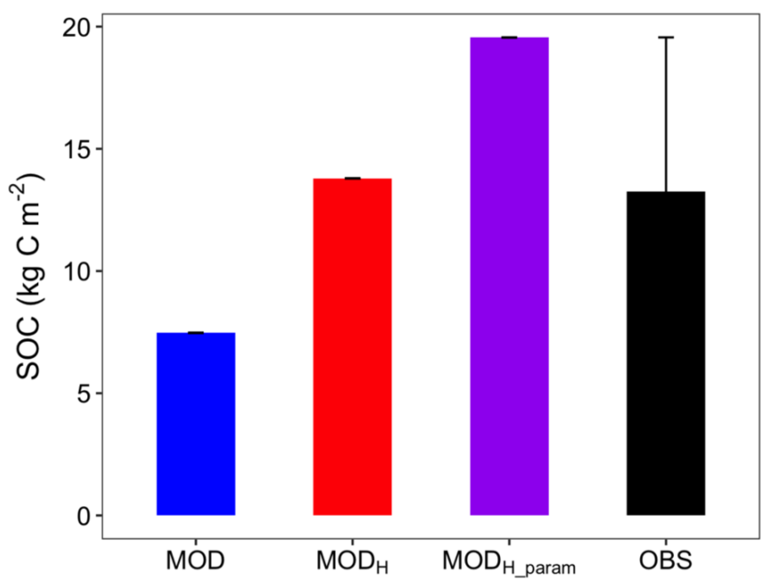

Figure S3 Comparison of the observed and modelled soil organic carbon (SOC) stocks. OBS: observation; MOD: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement using the Hanson model; MOD_{H_param}: model output after soil water potential improvement using the Hanson model and parameter adjustments.

A detailed report on the tuning of an ESM is valuable even if no new mechanisms were added. It helps to understand model performance and the thoughts behind the model development. For improving simulation of soil respiration, the authors had looked at the sensitivity to temperature, LAI, GPP, and relative contributions of roots and soil carbon, and tuned a bunch of parameters (Table 2 in page 5). A detailed analysis of the successes and fails of these tunings would be interesting. For example, I'd like to see how the improvement of SWP prediction affects plant physiology, photosynthesis, allocation, NPP (because NPP=Rh at equilibrium). These variables may change soil respiration.

Response: The reviewer provided an insightful suggestion. In the revised manuscript, we added the analyses of the effects of the improved SWP on photosynthesis, NPP, and carbon allocation to fine root, leaf and woody tissue (Fig. S7 and also see below). Results showed that the improved SWP generally increased all photosynthesis, NPP and carbon allocations to different tissues during the growing season. In addition, parameter adjustments further increased them.

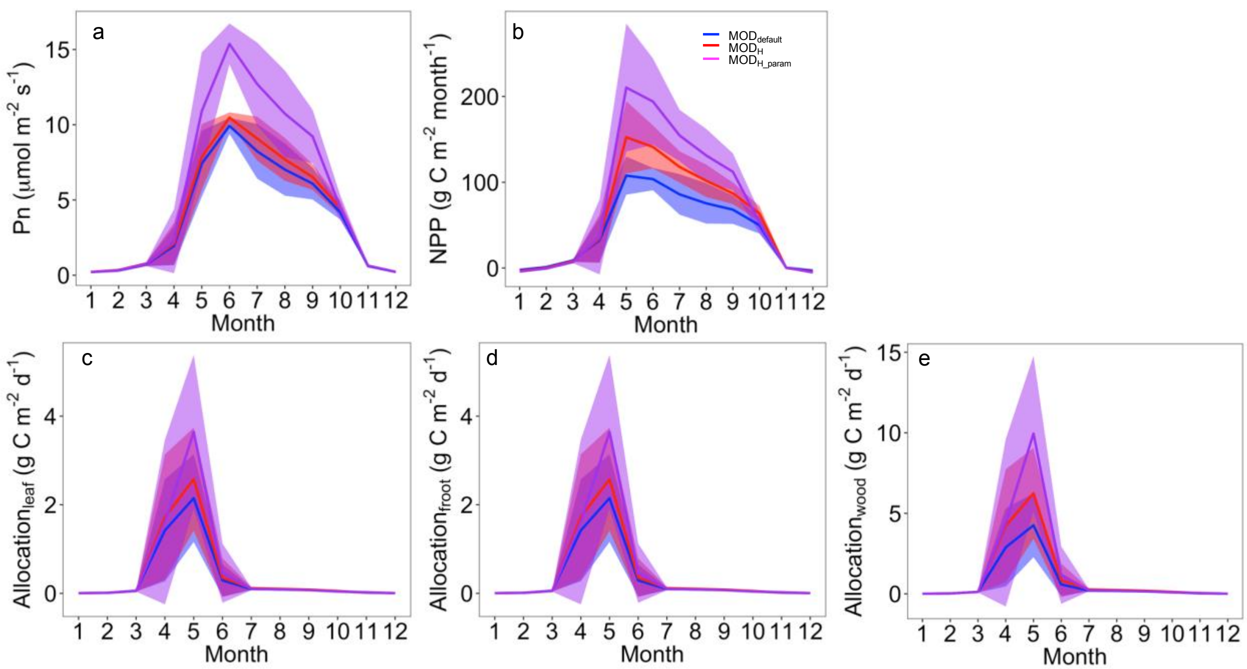

Figure S7 The annual mean cycles of photosynthesis (Pn), net primary production (NPP) and C allocations to fine root ($\mathbf{Allocation_{froot}}$), leaf ($\mathbf{Allocation_{leaf}}$) and woody tissue ($\mathbf{Allocation_{wood}}$). $MOD_{default}$: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement using the Hanson model; MOD_{H_param}: model output after soil water potential improvement using the Hanson model and parameter adjustments.

We added the description of these results in the revised manuscript as (page 10, lines 13 – 18):

"In addition, we analyzed changes in simulated evapotranspiration (ET), runoff, photosynthesis, net primary production, C allocations to fine roots, leaf and woody tissue in response to the

changes in the soil water scheme and parameters (Fig. S6, S7). The change in soil moisture scheme and parameter adjustments slightly increased ET and decreased runoff. Despite these slight changes, the model simulated ET generally fell within the observed range, with or without changes in soil water scheme and parameters (Fig. S6). The improved SWP and parameter adjustments generally increased all photosynthesis, NPP and carbon allocations to different tissues during the growing season (Fig. S7)."

Specifically, for water effects on soil heterotrophic respiration, the model uses two equations to link volumetric water content to heterotrophic respiration: VMC–>SWP and SWPRh. The second equation (SWPRh, Eq 9 in page 4) is much more critical than the first one for modeling heterotrophic respiration. It represents the knowledge of how soil moisture affects microbial physiology. It needs to be explored in detail if the goal of this research is to improve the simulation of soil respiration.

Response: We agree with the reviewer that the moisture modifier (ξ_W) is a critical factor in the model in determining how soil moisture affects microbial physiology. In the revised manuscript, we analyzed the effect of the improved SWP on ξ_W (Fig. S2b). The improved SWP increased ξ_W during the peak growing season, and reduced ξ_W during the non-growing season (Fig. S2), which was consistent with the changes in SWP (Fig. 3b). The changes in ξ_W, as well as GPP and SOC stocks, jointly determined the effect of the improved SWP on SR, as discussed above and in the revised manuscript.

The related revisions are shown below and in the text (page 8, lines 1 – 6; page 11, lines 3 – 14).

"The changes in annual SR and GPP (i.e., the differences between before and after the improved SWP simulation using the Hanson model) showed a linear relationship (Fig. S1). In addition, the improved soil water scheme using the Hanson model increased both the moisture modifiers of GPP and heterotrophic respiration (i.e., btran and ξ_W) during the peak growing season, and reduced ξ_W during the non-growing season (Fig. S2). While SOC when simulated by the model with different soil water schemes generally fell within the wide range of observations, the improved SWP simulations using the Hanson model increased SOC stocks (Fig. S3)."

"Constraining the SWP-VWC relationship with site-specific data and using the Hanson model instead of the ELMv0 default model (Fig. 1) significantly improved the model representation of SWP (Fig. 3) and annual SR (Fig. 2a). The improvements in model fits were due to changes in GPP, SOC stocks, and the moisture modifier on heterotrophic respiration (Figs. S1 – S3). First, the default ELMv0 underestimated GPP (Fig. 2b), as in a recent study where CLM4.5 significantly underestimated GPP at a coniferous forest in northeastern United States (Duarte et al., 2017). GPP affects the substrate supply for SR, as evidenced by the close relationship between changes in SR and GPP (Fig. S1), which is consistent with experimental evidence showing GPP can directly affect the magnitude of root respiration (Craine et al., 1999; Högberg et al., 2001; Wan and Luo, 2003; Verburg et al., 2004; Gu et al., 2008). Second, the changed soil moisture scheme increased the moisture modifier (ξ_W) on heterotrophic respiration during the peak-growing season, and decreased it during the non-growing season (Fig. S2), which is consistent with the trend of changes in SWP (Fig. 3). In addition, the changed soil

moisture scheme also increased the simulated SOC stock, the substrate for heterotrophic respiration (Fig. S3). These changes together resulted in the improvement of simulated SR."

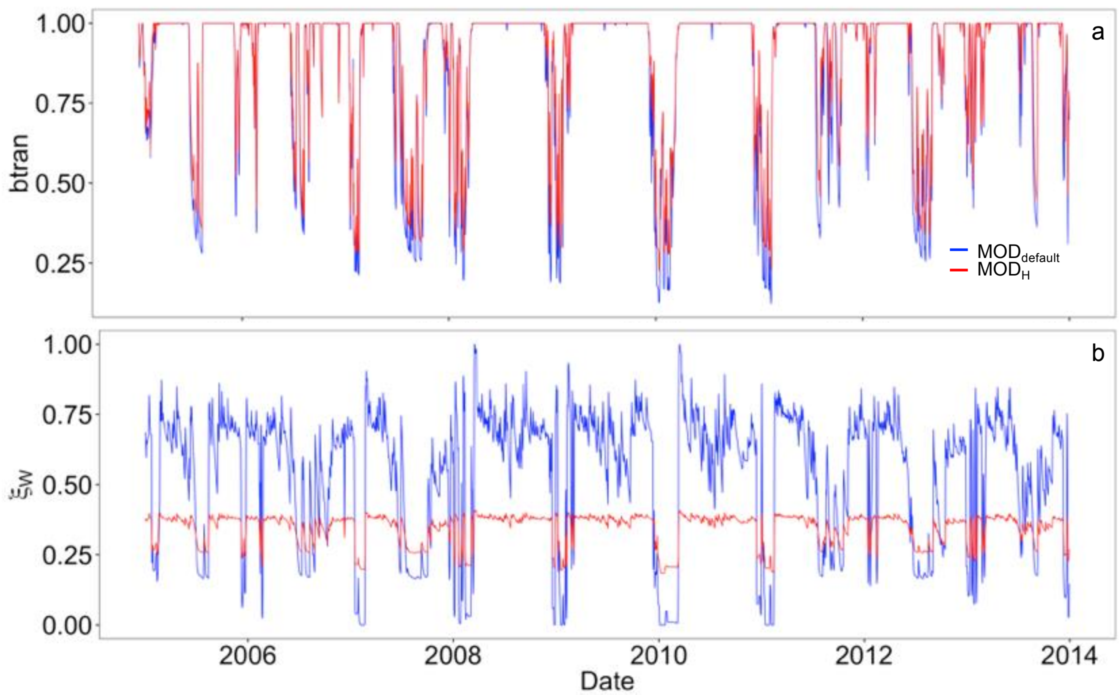

Figure S2 Impact of the changed SWP on the moisture modifiers of GPP (btran, a) and heterotrophic respiration (ξw, b). $MOD_{default}$: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement using the Hanson model.

Short comment 1:

Dear authors,
in my role as Executive editor of GMD, I would like to bring to your attention our Editorial version 1.1:

http://www.geosci-model-dev.net/8/3487/2015/gmd-8-3487-2015.html

This highlights some requirements of papers published in GMD, which is also available on the GMD website in the 'Manuscript Types' section:

http://www.geoscientific-model-development.net/submission/manuscript_types.html

In particular, please note that for your paper, the following requirement has not been met in the Discussions paper:

• "The main paper must give the model name and version number (or other unique identifier) in the title."

Even if this is not a strict requirement for evaluation paper, we like to encourage authors to provide also the version number of the evaluated model, as usually evaluation results depend on model version.

Additionally, please not, that GMD is encouraging authors to provide a persistent access to the exact version of the source code used for the model version presented in the paper. As explained in https://www.geoscientific-modeldevelopment.net/about/manuscript_types.html the preferred reference to this release is through the use of a DOI which then can be cited in the paper. For projects in GitHub (such as thee E3SM Land Model) a DOI for a released code version can easily be created using Zenodo, see https://guides.github.com/activities/citable-code/ for details.

Yours,
Astrid Kerkweg

Response: We appreciate the comments. We revised the title to include the model name and version number. The revised title is *"Evaluating the E3SM Land Model version 0 (ELMv0) at a temperate forest site using flux and soil water measurements"*. We also provided the link to the model.

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Evaluating the E3SM Land Model version 0 (ELMv0) at a temperate forest site using flux and soil water measurements

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Abstract. Accurate simulations of soil respiration and carbon dioxide (CO_2) efflux are critical to project global biogeochemical cycles and the magnitude of carbon (C) feedbacks to climate change in Earth system models (ESMs). Currently, soil respiration is not represented well in ESMs, and few studies have attempted to address this deficiency. In this study, we evaluated the simulation of soil respiration in the Energy Exascale Earth System Model (E3SM) Land Model version 0 (ELMv0) using long-term observations from the Missouri Ozark AmeriFlux (MOFLUX) forest site in the central U.S. Simulations using the default model parameters significantly underestimated annual soil respiration and gross primary production, while underestimating soil water potential during peak growing seasons and overestimating it during non-growing seasons. A site-specific soil water retention curve significantly improved modelled soil water potential, gross primary production and soil respiration. However, the model continued to overestimate soil respiration during non-growing seasons. One potential reason may be that the current model does not adequately represent the seasonal cycle of microbial organisms and soil macroinvertebrates, which have high biomass and activity during peak growing seasons and tend to be dormant during non-growing seasons. Our results confirm that modelling soil respiration can be significantly improved by better model representations of the soil water retention curve.

1 Introduction

Globally, soils store over twice as much carbon (C) as the atmosphere (Chapin III et al., 2011). Soil respiration (SR) is the second largest C flux between terrestrial ecosystems and the atmosphere (Luo and Zhou, 2006). An accurate simulation of SR is critical for projecting terrestrial C status, and therefore climate change, in Earth system models (ESMs) (IPCC, 2013).

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Despite significant experimental data accumulation and model development during the past decades, simulations of soil CO_2 efflux to the atmosphere still have a high degree of uncertainty (Friedlingstein et al., 2006; Jones et al., 2013; Todd-Brown et al., 2013; Todd-Brown et al., 2014; Tian et al., 2015), calling for comprehensive assessments of model performance against observational data.

To assess the performance of ESMs, different types of data can be used. For example, using atmospheric CO_2 observations, eddy covariance measurements and remote sensing images, Randerson et al. (2009) found that two ESMs underestimated net C uptake during the growing season in temperate and boreal forest ecosystems, primarily due to the delays in the timing of maximum leaf area in the models. By comparing remote sensing estimations from the Moderate Resolution Imaging Spectroradiometer and flux tower datasets, Xia et al. (2017) found that better representations of processes controlling monthly maximum gross primary productivity (GPP) and vegetation C use efficiency (CUE) improved the ability of models to predict the C cycle in permafrost regions.

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Despite the significance of large global SR fluxes, SR has rarely been evaluated in ESMs using long-term observations. Among the factors that influence SR, soil water potential (SWP) provides a unified measure of the energy state of soil water that limits the growth and respiration of plants and microbes. Unlike soil temperature (ST) or soil volumetric water content (VWC), however, SWP is difficult to directly monitor in the field. Accurate estimation of SWP largely relies on the soil water retention curve (i.e., the relationship between VWC and SWP), which is highly specific to soil properties (Childs, 1940; Clapp and Hornberger, 1978; Cosby et al., 1984; Tuller and Or, 2004; Moyano et al., 2013). Site-level data have been used to evaluate model representations of other processes, such as phenology, net primary production (NPP), transpiration, leaf area index (LAI), water use efficiency, and nitrogen use efficiency (Richardson et al., 2012; De Kauwe et al., 2013; Walker et al., 2014; Zaehle et al., 2014; Mao et al., 2016; Duarte et al., 2017; Montané et al., 2017). In Powell et al. (2013), the only aspect influencing the modelling of SR was the sensitivity of SR to VWC in an Amazon forest, but the study resulted in no improvements to simulated SR. Here, we focus on improving simulations by using site-specific measurements to assess multiple factors influencing SR.

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We will evaluate the simulation of SR step by step. We assessed underlying mechanisms in the Energy Exascale Earth System Model (E3SM) Land Model version 0 (ELMv0) by using intensive observations at the Missouri Ozark AmeriFlux (MOFLUX) forest site in the central U.S. We first evaluated the effects of two abiotic factors, ST and SWP, on the simulation of SR. Then we evaluated the effects of biotic factors, such as GPP, LAI and Q_{10} of heterotrophic respiration, on the simulation of surface CO_2 efflux to the atmosphere.

2 Materials and Methods

2.1 Study site and measurements

The MOFLUX site is located in the University of Missouri's Thomas H. Baskett Wildlife Research and Education Area (latitude 38º44'39"N, longitude 92º12'W). The mean annual precipitation is 1083 mm, while minimum and maximum monthly mean temperatures are −1.3 ºC (January) and 25.2 ºC (July), respectively. The site is a temperate, upland oak-hickory forest, with major tree species consisting of white oak (*Quercus alba* L.), black oak (*Q. velutina* Lam.), shagbark hickory (*Carya ovata* (Mill.) K. Koch), sugar maple (*Acer saccharum* Marsh.), and eastern red cedar (*Juniperus virginiana* L.) (Gu et al., 2016; Wood et al., 2017). The dominant soils are the Weller silt loam and the Clinkenbeard very flaggy clay loam (Young et al., 2001).

Ecosystem C, water and energy fluxes, SR, LAI and supporting meteorological measurements were initiated in June 2004 (Gu et al., 2016). Soil respiration was measured within the ecosystem flux tower footprint using non-flow through non-steady state auto-chambers. From 2004 through 2013, SR was measured using eight automated, custom-built chambers (ED system; Edwards and Riggs, 2003; Gu et al., 2008) coupled with an infrared gas analyzer (LI-820 Li-Cor Inc., Lincoln, Nebraska). In 2013, this system was replaced with 16 auto-chambers operated using the closed-path system (model LI-8100; Li-Cor Inc., Lincoln, Nebraska). The two systems (ED and Li-8100) were operated side-by-side for several weeks in 2010 and found to produce comparable responses (Paul Hanson, personal communication). Half-hourly SR time series were generated to coincide with the ecosystem flux data set by averaging those chambers sampled in the corresponding averaging period. Net ecosystem CO_2 exchange (NEE) was measured on a 32-m walk-up scaffold tower (Gu et al., 2016). A soil temperature profile sensor (model STP01, HuksefluxUSA, Inc., Center Moriches, NY) measured at 5 depths down to 0.5 m. Soil VWC was measured using water content reflectometers (model CS616, Campbell Scientific Inc., Logan UT) installed beneath each soil chamber. All the data were recorded at half-hourly intervals, which were integrated over time to obtain daily and annual fluxes.

2.2 Ecosystem C flux partitioning

Flux-tower GPP was estimated from measured NEE. To reduce biases resulting from individual methods, three NEE-partitioning approaches were employed. The average and variation of the three methods were used to evaluate the model-simulated GPP. In the first two methods, ecosystem respiration (ER) was estimated from nighttime NEE and extrapolated to daytime, and daytime GPP was calculated from NEE and the extrapolated ER (Reichstein et al., 2005). The only difference between the two methods was whether to exclude night-time data under non-turbulent conditions. In the third method, GPP was estimated by fitting the light-response curve between NEE and radiation (Lasslop et al., 2010). All the partitioning calculations were conducted using the R package *REddyProc* (Reichstein et al., 2017).

2.3 Model description

The ELMv0 used in this study is structurally equivalent to the Community Land Model 4.5 (CLM 4.5), which includes coupled carbon and nitrogen cycles (Oleson et al., 2013). In ELMv0, the soil biogeochemistry can be simulated with one-layer or multi-layer converging trophic cascade (CTC, i.e., CLM-CN) decomposition model. We used the vertically-resolved CTC decomposition in this study. In the model, SR was calculated by different CO_2 emission components (Oleson et al., 2013):

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Deleted: The E3SM includes coupled carbon and nitrogen cycles, with 10 belowground layers in the biogeochemical module.

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$$SR = R_A + R_H \quad \text{Eq. (1)}$$

$$R_A = R_M + R_G \quad \text{Eq. (2)}$$

$$R_M = R_{livecroot} + R_{froot} \quad \text{Eq. (3)}$$

$$R_{liveroot} = [N]_{livecroot} R_{base} R_{q10}^{(T_{2m}-20)/10} \quad \text{Eq. (4)}$$

$$R_{froot} = \sum_{j=1}^{10} [N]_{froot} rootfr_j R_{base} R_{q10}^{(T_{2m}-20)/10} \quad \text{Eq. (5)}$$

$$R_G = 0.3 C_{new\_root} \quad \text{Eq. (6)}$$

$$R_H = \sum_{j=1}^{10} \sum_{i=1}^{4} SOC_{ij} k_i rf_i \xi_T \xi_W \xi_O \xi_D \xi_N \quad \text{Eq. (7)}$$

where R_A and R_H are belowground autotrophic and heterotrophic respiration, respectively. R_A is the sum of root maintenance (R_M) and growth respiration (R_G). $R_{livecroot}$ and R_{froot} are maintenance respiration of live course root and fine root. $[N]_{livecroot}$ and $[N]_{froot}$ are nitrogen content of live coarse and fine roots. R_{base} is the base maintenance respiration at 20 ºC. R_{q10} which equals 2, is the temperature sensitivity of maintenance respiration. T_{2m} is the air temperature at 2 m. C_{new_root} is the new root growth C. R_H is the sum of heterotrophic respiration of four SOC pools with different turnover rates (Oleson et al., 2013) in the 10 soil layers. The parameters k_i and rf_i are the turnover rate and respiration fraction of the i^{th} pool. ξ_T, ξ_W, ξ_O, ξ_D, ξ_N are environmental modifiers of soil temperature, soil water content, oxygen, depth and nitrogen for each layer, respectively. A detailed description of the environmental modification can be found in Oleson et al. (2013). Briefly, the temperature and water modifiers were:

$$\xi_T = Q_{10}^{\left(\frac{T_{soil}-T_{ref}}{10}\right)} \quad \text{Eq. (8)}$$

$$\xi_W = \begin{cases} 0 & for\ \Psi < \Psi_{min} \\ \frac{log(\Psi_{min}/\Psi_m)}{log(\Psi_{min}/\Psi_s)} & for\ \Psi_{min} \le \Psi \le \Psi_{max} \\ 1 & for\ \Psi > \Psi_{max} \end{cases} \quad \text{Eq. (9)}$$

where Q_{10} is the temperature sensitivity (the default value is 1.5), T_{ref} is the reference temperature (25 ºC). Ψ_m is the matric water potential, Ψ_{min} is the lower limit for matric potential, and Ψ_s is the matric water potential under saturated conditions.

The ELMv0 is a grid-based model. To assess it using site-level observations, we used a point-run framework which allows the model to simulate individual sites (Mao et al., 2016). Single-point runs forced with site-level measurements have a long history to evaluate model representations of phenology, NPP, transpiration, LAI, water use efficiency, and nitrogen use efficiency (Richardson et al., 2012; De Kauwe et al., 2013; Walker et al., 2014; Zaehle et al., 2014; Mao et al., 2016; Duarte et al., 2017; Montané et al., 2017). With site-specific forcing, a 200-year accelerated decomposition spin-up was performed, followed by a 200-year normal spin-up, before the transient simulation was performed from 1850 to 2013. The vegetation was set as 100% temperate deciduous forest.

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2.4 Soil water retention curve

Soil water potential values for the Weller soils (https://soilseries.sc.egov.usda.gov/OSD_Docs/W/WELLER.html) were estimated from observed VWC and soil water retention curves that were developed for the site. To derive the soil water retention curves, soil samples were collected in the area of the flux tower base at two depths: 0 to 30 cm and below 30 cm. Samples were evaluated periodically for soil water potential using a dewpoint potentiometer (Decagon Devices, Model WP4C) as they dried over time (Hanson et al., 2003).

In the ELMv0, the SWP was calculated from VWC based on the Clapp & Hornberger model (Clapp and Hornberger, 1978), in which the SWP-VWC relationship was expressed as

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$$\Psi_m = \Psi_s \left(\frac{\theta}{\theta_s}\right)^{-B} \qquad \text{Eq. (10)}$$

where θ and Ψ_m are the VWC and matric potential (MPa); and θ_s and Ψ_s are VWC and matric potential under saturated conditions, and B is a parameter to determine the shape of the SWP-VWC relationship. In the ELMv0, all parameters were calculated from the fraction of organic matter (f_{om}), clay content (f_{clay}; %) and sand content (f_{sand}; %) (Cosby et al., 1984; Lawrence and Slater, 2008), where

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$$\Psi_s = -\left((1 - f_{om}) \times 10 \times 10^{1.88-0.0131 f_{sand}} + 10.3 f_{om}\right) \qquad \text{Eq. (11)}$$

$$\theta_s = \left((1 - f_{om}) \times (0.489 - 0.00126 f_{sand}) + 0.9 f_{om}\right) \qquad \text{Eq. (12)}$$

$$B = (1 - f_{om}) \times \left(2.91 + 0.159 f_{clay}\right) + 2.7 f_{om} \qquad \text{Eq. (13)}$$

In addition to the Clapp & Hornberger model, four other empirical models (Brooks and Corey, 1964; van Genuchten, 1980; Fredlund and Xing, 1994; Hanson et al., 2003) were also used to fit the SWP curve against VWC (Table 1, Figure 1).

Field Code Changed

In the Brooks & Corey model, the SWP-VWC relationship was expressed as

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = \begin{cases} \left(\frac{\Psi_b}{\Psi_m}\right)^{\lambda} & \Psi_m > \Psi_b \\ 1 & \Psi_m \le \Psi_b \end{cases} \qquad \text{Eq. (14)}$$

where θ_r and θ_s are the residual and saturated water contents, respectively, θ and Ψ_m are measured VWC and matric potential (MPa), Ψ_b is a parameter related to the soil matric potential at air entry, and λ is related to the soil pore size distribution (Brooks and Corey, 1964).

In the Fredlund & Xing model, the SWP-VWC relationship was described as

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[\frac{1}{\ln\left(e + (\Psi_m/a)^n\right)}\right]^m \qquad \text{Eq. (15)}$$

where *a*, *n* and *m* are parameters determining the shape of the soil water characteristic curve (Fredlund and Xing, 1994).

In the Hanson model (Hanson et al., 2003), soil matric potential was modelled by a double exponential function:

$$\Psi_m = -a^{b\theta^c} - d \qquad \text{Eq. (16)}$$

where *a*, *b*, *c* and *d* are fitted parameters.

In the van Genuchten model, the SWP-VWC relationship was described as

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[\frac{1}{1 + (\alpha \Psi_m)^n}\right]^{(1-1/n)} \qquad \text{Eq. (17)}$$

where α (MPa^{-1}) and n are parameters that determine the shape of the soil-water curve (van Genuchten, 1980).

In addition to the default SWP-VWC relationship in the ELMv0, all the five empirical models were parameterized using non-linear fitting against measured VWC and SWP data from the study site. For the calibration of the Clapp & Hornberger model, instead of using the hard-coded parameters in Eq. 11-13, we calibrated the three parameters (i.e., Ψ_m, θ_s and Ψ_s) in the Clapp & Hornberger model (Eq. 10). The root-mean-square error (RMSE) was used to select the best model representing the SWP-VWC relationship, where smaller RMSE implies a better fit to observational data. The best-fit model was used in two ways. First, it was used to calculate the "observed" SWP from monitored VWC in the field. Second, it was implemented in the ELMv0 to replace the default SWP model in order to improve the SWP simulation.

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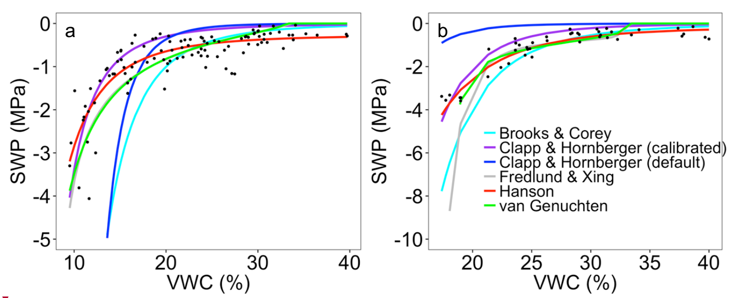
2.5 Evaluation of SR in the model

The evaluation of SR was conducted step by step. We first compared observations with the model default output of SR and related factors, including ST, SWP, GPP, and LAI. Thereafter, we attempted to improve the simulation of these factors in order to improve the overall SR simulation by (i) implementing the best-fit SWP-VWC relationship, and (ii) modifying model parameters related to GPP, LAI and SR. GPP-related parameters included the specific leaf area (SLA) at the top of canopy and the fraction of leaf nitrogen in the RuBisCO enzyme. LAI-related parameters included the number of days to complete leaf fall during the end of growing season, the critical day length for senescence (i.e., the length of the day when leaves start to senesce), and a parameter α that was used to produce a linearly-increasing rate of litterfall. In addition, the Q_{10} of heterotrophic respiration was also modified. Because the parameter modification was dependent on the evaluation steps, how the parameters were modified is presented in the Results section.



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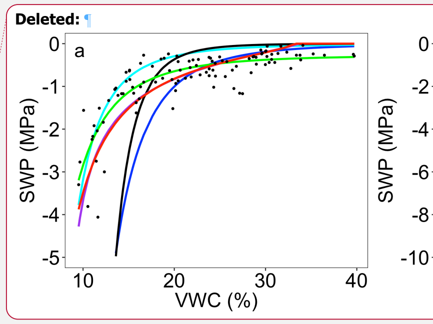

Figure 1: Observed (black dots) and simulated relationship between soil water potential (SWP) and volumetric water content (VWC) by the different models at two soil layers: (a) 0 to 30 cm and (b) below 30 cm.

3 Results

For the upper 30 cm of soil, the ELMv0 simulations using the default Clapp and Hornberger model tended to underestimate the SWP when VWC was less than 15% (Fig. 1a), while SWP rapidly approached zero when VWC was greater than 25% (Fig. 1a). For soil below 30 cm, the ELMv0 showed a consistent overestimation of SWP when VWC exceeded 15% (Fig. 1b). The default ELMv0 showed relatively high RMSE for both soil layers, indicating that the SWP-VWC relationship was not well simulated in the ELMv0 (Table 1). Although the Clapp & Hornberger model performed better by using parameters from non-linear fitting, its performance was not as good as the Hanson and the van Genuchten models (Table 1, Fig. 1). The Hanson model was the best-fit model for the MOFLUX site, showing the smallest RMSE and AIC values for both soil layers (Table 1, Fig. 1), and was therefore implemented in ELMv0 to calculate SWP from measured VWC.

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Table 1. Root-mean-square-error (RMSE) and Akaike Information Criterion (AIC) of different models in simulating the SWP-VWC relationship for the soil in the MOFLUX site at two depths: 0 to 30 cm and below 30 cm.

	< 30 cm		> 30 cm	
Model	RMSE	AIC	RMSE	AIC
Clapp & Hornberger (default ELMv0)	4.25	157.82	1.33	18.51
Brooks & Corey	3.91	151.05	1.13	13.51
Clapp & Hornberger (calibrated)	0.53	-61.03	0.51	-23.43
Fredlund & Xing	0.51	-63.15	2.43	47.13
Hanson	0.41	-86.07	0.34	-38.98
van Genuchten	0.50	-65.53	0.36	-36.61

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The ELMv0 default run significantly underestimated both annual SR and GPP (Fig. 2). In addition, the simulated SR had smaller interannual variability compared to the observations. The model was not able to simulate the steep drop of SR or GPP during the extreme drought in 2012. The simulations of ST and SWP were isolated to analyse their contributions to model performance. Whereas the model simulated ST well at 10 cm depth (Fig. 3a), it tended to underestimate SWP when water is limiting and to overestimate SWP otherwise (Fig. 3b). Implementing the data-constrained Hanson model significantly improved the simulation of SWP, showing a greater R^2 and a much smaller RMSE than that of the default run (Fig. 3b). After improving the simulation of SWP, the model better matched the observed annual SR and GPP (Fig. 2). The mean annual simulations of SR and GPP fell into the 1 sigma (i.e., standard deviation) of observations (inserted plot in Fig.

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2). The changes in annual SR and GPP (i.e., the differences between before and after the improved SWP simulation using the Hanson model) showed a linear relationship (Fig. S1). In addition, the improved soil water scheme using the Hanson model increased both the moisture modifiers of GPP and heterotrophic respiration (i.e., btran and ξ_W) during the peak growing season, and reduced ξ_W during the non-growing season (Fig. S2). While SOC when simulated by the model with different soil water schemes generally fell within the wide range of observations, the improved SWP simulations using the Hanson model increased SOC stocks (Fig. S3).

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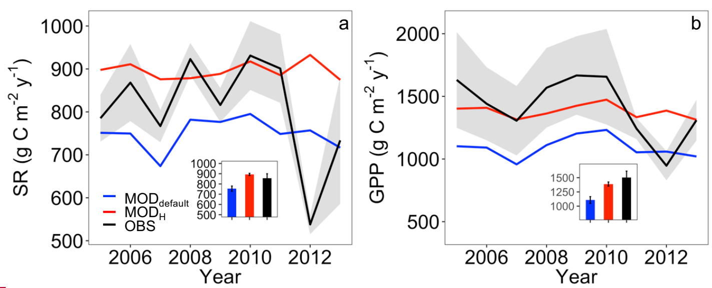

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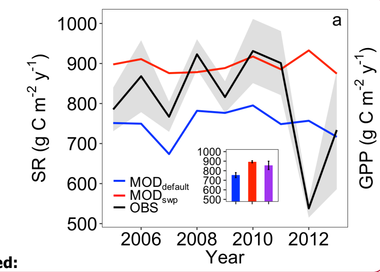

Figure 2: Annual soil respiration (SR) and gross primary production (GPP). Blue and red lines are model outputs before ($MOD_{default}$) and after (MOD_H) soil water potential improvement, respectively. Black lines and grey area are the observed (OBS) mean and 1 sigma (i.e., standard deviation) range, which were calculated from eight field replications for SR, and from three different net ecosystem exchange partitioning methods for GPP. The inserted bar plots are mean annual average ± 1 sigma across 2005-2011.

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Despite the improved simulation of SR, the model still underestimated SR and GPP during peak growing seasons when SR and GPP were high, and overestimated them during non-growing seasons (Figs. 4, S4). In other words, though the improved simulation of SWP increased SR and GPP during peak growing seasons, the model still showed systematic errors. We attempted to improve the seasonal simulations of SR, GPP and LAI by modifying several related parameters (Table 2). Using measurements of C and energy fluxes from the MOFLUX site, Lu et al. (2018) calibrated a polynomial surrogate model of the ELMv0. Based on their results, we modified two parameters, i.e., the SLA at the canopy top from 0.03 to 0.01, and the fraction of leaf nitrogen in the RuBisCO enzyme from 0.1007 to 0.12.

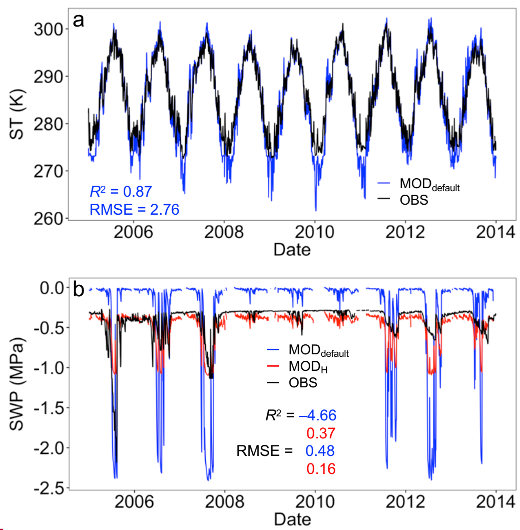

Figure 3: Daily soil temperature (ST) and soil water potential (SWP) at 10 cm. Blue and red lines/dots are model outputs before ($MOD_{default}$) and after (MOD_H) soil water potential improvement, respectively. R^2 and RMSE are shown in corresponding colours. Extremely low SWP values due to frozen soil water are not shown.

Table 2. Modified parameters to better simulate gross primary production (GPP) and leaf area index (LAI) at the MOFLUX site in the ELMv0.

Parameter name (unit*)	Parameter description	Default model value	Tuned values
slatop	Specific leaf area at top of canopy	0.03	0.01
flnr	Fraction of leaf nitrogen in RuBisCO enzyme	0.1007	0.12
ndays_off (d)	Number of days to complete leaf offset	15	45
Crit_dayl (s)	Critical day length for senescence	39300	43200
α	To control the rate coefficient r_{xfer_off} to produce a linearly-increasing litterfall rate	2	10

*slatop, flnr and α are unitless

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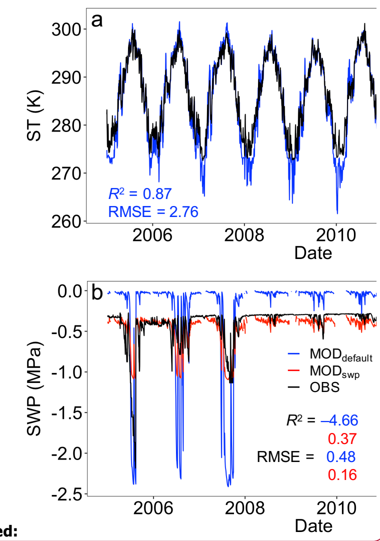

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Comparing the simulated LAI with the observations (Fig. 4), we found that the parameter *ndays_off* (number of days to complete leaf offset) in the ELMv0 was too short (default value = 15 days) for the MOFLUX site. Thus, we reset the value of *ndays_off* to 45 days. We also modified the values of two additional parameters, i.e., *crit_dayl* and α correspondingly (Table 2). Parameter *crit_dayl* (the critical day length for senescence, units: second) triggers the leaf falling during the end of the growing season. Parameter (α) is used to produce a linearly-increasing litterfall rate. Results showed that the ELMv0 with both the default and improved SWP by the Hanson model overestimated the maximum LAI (Fig. 4a). The adjustment of the aforementioned five parameters (Table 2) significantly reduced the LAI to within a more reasonable range (Fig. 4a). The parameter changes further increased the simulated GPP and SR during the peak growing season, in addition to the improvement by the adjusted SWP (Fig. 4b, c). However, all modifications of the ELMv0 still overestimated SR during the non-growing season, resulting in significant overestimation of annual SR fluxes (Fig. S5a). After the parameter adjustments, the annual GPP flux was still within the observed range (Fig. S5b).

In addition, we analyzed changes in simulated evapotranspiration (ET), runoff, photosynthesis, net primary production, C allocations to fine roots, leaf and woody tissue in response to the changes in the soil water scheme and parameters (Fig. S6, S7). The change in soil moisture scheme and parameter adjustments slightly increased ET and decreased runoff. Despite these slight changes, the model simulated ET generally fell within the observed range, with or without changes in soil water scheme and parameters (Fig. S6). The improved SWP and parameter adjustments generally increased all photosynthesis, NPP and carbon allocations to different tissues during the growing season (Fig. S7).

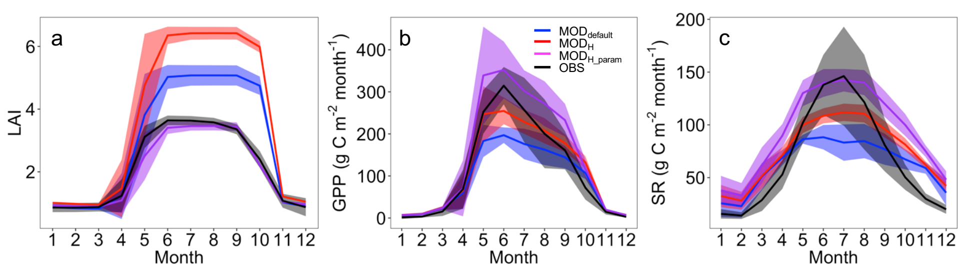

Figure 4 The annual mean cycles of leaf area index (LAI), gross primary production (GPP) and soil respiration (SR). OBS: observation; $MOD_{default}$: model output before soil water potential improvement; MOD_H: model output after soil water potential improvement by the Hanson model; MOD_{H_param}: model output after soil water potential improvement by the Hanson model and parameter adjustments.

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4 Discussion

4.1 Effect of SWP on annual SR

Constraining the SWP-VWC relationship with site-specific data and using the Hanson model instead of the ELMv0 default model (Fig. 1) significantly improved the model representation of SWP (Fig. 3) and annual SR (Fig. 2a). The improvements in model fits were due to changes in GPP, SOC stocks, and the moisture modifier on heterotrophic respiration (Figs. S1 – S3). First, the default ELMv0 underestimated GPP (Fig. 2b), as in a recent study where CLM4.5 significantly underestimated GPP at a coniferous forest in northeastern United States (Duarte et al., 2017). GPP affects the substrate supply for SR, as evidenced by the close relationship between changes in SR and GPP (Fig. S1), which is consistent with experimental evidence showing GPP can directly affect the magnitude of root respiration (Craine et al., 1999; Högberg et al., 2001; Wan and Luo, 2003; Verburg et al., 2004; Gu et al., 2008). Second, the changed soil moisture scheme increased the moisture modifier (ξ_W) on heterotrophic respiration during the peak-growing season, and decreased it during the non-growing season (Fig. S2), which is consistent with the trend of changes in SWP (Fig. 3). In addition, the changed soil moisture scheme also increased the simulated SOC stock, the substrate for heterotrophic respiration (Fig. S3). These changes together resulted in the improvement of simulated SR.

The simulation of SWP in the default ELMv0 was poor compared with that of ST (Fig. 2), which may be a common issue in ESMs. For example, using a reduced-complexity model, Todd-Brown et al. (2013) demonstrated that the spatial variation in soil C in most ESMs is primarily dependent on C input (i.e., NPP) and ST, showing R^2 values between 0.62 and 0.93 for 9 of 11 ESMs. However, the same reduced-complexity model, driven by observed NPP and ST, can only explain 10% of the variation in the Harmonized World Soil Database observational database (Todd-Brown et al., 2013). These previous results indicate that other important factors affecting soil C dynamics, in addition to NPP and ST, are inadequately simulated in ESMs (Powell et al., 2013; Reyes et al., 2017). Powell et al. (2013) showed that differential sensitivity of SR to VWC in several ESMs using observations in two Amazon forests. Our analyses in this study indicate that improving the modelled SWP can significantly improve SR simulations. Thus, we argue that the SWP simulation in ESMs should be calibrated carefully with observations, and/or by using different model representations of the SWP-VWC relationship.

In this study, we derived better SWP-VWC relationship by using non-linear fitting, primarily because of the availability of soil moisture retention curve data. It is an efficient method when site-level data is available, but it is not realistic to calibrate the water retention curve for every site. The SWP-VWC relationship is dependent on soil texture (Clapp and Hornberger, 1978; Cosby et al., 1984; Tuller and Or, 2004), so building relationships between model parameters and soil texture may allow efficient extrapolations of site-level measurements to regional and global scales.

Parameters in the default Clapp & Hornberger model used in the ELMv0 were derived from synthesizing data across soil textural classes (Clapp and Hornberger, 1978; Cosby et al., 1984; Lawrence and Slater, 2008). The data were derived from over 1,000 soil samples from 11 USDA soil textural classes (Holtan et al., 1968; Rawls et al., 1976). The dependence of model parameters on soil texture were derived from a regression of these 11 data points, i.e., the mean parameter values of

Deleted: Figure 6 The annual mean cycles of leaf area index (LAI), gross primary production (GPP) and soil respiration (SR). OBS: observation; $MOD_{default}$: model output before soil water potential improvement; MOD_{swp}: model output after soil water potential improvement; MOD_{swp_param}: model output after soil water potential improvement and parameter modification.

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11 soil textural classes against the sand or clay fractions (Cosby et al., 1984). Because no actual sand or clay content of soil samples was reported in the original databases (i.e., only the soil textural classes were reported), the sand and clay fractions used for the regression were obtained from midpoint values of each textural class (Clapp and Hornberger, 1978; Cosby et al., 1984). One potential issue is that soil samples in the same textural classes can have different sand and clay contents and SWP-VWC relationships, which may not be fully represented when they are grouped together. A re-analysis of an updated SWP-VWC database, with actual sand and clay content measurements, may enable improved relationships between model parameters and soil texture in the water retention model.

In addition, different empirical models have been developed to describe the SWP-VWC relationship (Brooks and Corey, 1964; Clapp and Hornberger, 1978; van Genuchten, 1980; Fredlund and Xing, 1994; Hanson et al., 2003). These models could be evaluated with an updated SWP-VWC database, and the selected best-fit model(s) could be used to calculate SWP in the field from continuously monitored VWC (e.g., from the AmeriFlux network) on different spatial and temporal scales. A new field SWP-VWC database at different scales could be used as a benchmark to improve simulations of soil water and biogeochemical processes in ESMs.

Moreover, we also explored whether the calibrated Clapp & Hornberger model can lead to similar improvements with the Hanson model (Fig. S8). Generally, both the Hanson model and the calibrated Clapp & Hornberger model improved the simulation of GPP and SR in the ELM, in comparison with the default run (Fig. S8). The ELMv0 with the Hanson model consistently produced higher GPP and SR than that with the calibrated Clapp & Hornberger model. In comparison with the observations, the modelled SR generally fell within the 1 sigma (i.e., standard deviation) range of observations, by using both the Hanson model and the calibrated Clapp & Hornberger model. However, the modelled GPP with the calibrated Clapp & Hornberger model was still lower than the observations. Given the order of the goodness-of-fit of the SWP-VWC relationship was default Clapp & Hornberger model < calibrated Clapp & Hornberger model < calibrated Hanson model (Table 1), these results further support the conclusion that better representations of SWP can improve the simulations of carbon processes. Therefore, throughout the remainder of this manuscript, we used the Hanson model to represent the SWP-VWC relationship.

4.2 Representation of seasonal and interannual variabilities of SR in the ELMv0

Although the simulation of the SWP using the Hanson model improved the representation of both annual SR and GPP, the model continued to overestimate SR during the non-growing season (Figs. 4), resulting in significant overestimations of the annual SR fluxes (Fig. S5). In addition, no matter which SWP simulations were used, the ELMv0 had smaller interannual variability than the observations (Fig. 2). Specifically, the model was not able to capture the steep decreases in GPP and SR in the extreme drought year (i.e., 2012). These results indicate that the current model structure is not sensitive enough to environmental changes. A few potential reasons may contribute to the underestimated seasonal and interannual variability. In

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the ELMv0, heterotrophic respiration contributed a majority proportion (i.e., over 85%) to total SR during non-growing seasons (Fig. 5), suggesting that the overestimation of SR during these seasons was primarily due to the biased heterotrophic respiration simulation. A potential reason for the biased heterotrophic respiration simulation may be related to the temperature sensitivity (Q_{10}). Theoretically, a higher Q_{10} can result in greater seasonal variability of SR (Fig. S9). Compared to relatively small Q_{10} values, a larger Q_{10} can lead to lower heterotrophic respiration when temperature is below the reference temperature, and greater heterotrophic respiration when temperature is above the reference (Fig. S9). In the ELMv0, the reference temperature is 25 ºC and the Q_{10} of heterotrophic respiration is 1.5 (Oleson et al., 2013). A previous study derived a much greater Q_{10} value (i.e., 2.83) when the parameters were calibrated with data from another temperate forest (Mao et al., 2016). We hypothesized that the Q_{10} value of 1.5 may be too small for the MOFLUX site. We arbitrarily increased Q_{10} from 1.5 to 2.5, but there were minimal effects on the SR simulation (Fig. S10). This indicates that modifying the temperature sensitivity of heterotrophic respiration may not improve the modelled representation of seasonality of SR in the ELMv0.

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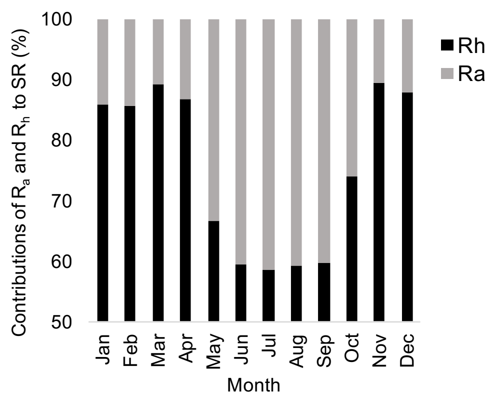

Figure 5: Modelled contributions of autotrophic (R_a) and heterotrophic (R_h) respiration to total soil respiration (SR).

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Another potential reason for the biased heterotrophic respiration simulation may be that the seasonality of microbial organisms was not adequately represented in the model. Like most ESMs, the ELMv0 represents soil C dynamics using linear differential equations and assumes that SR is a substrate-limited process in the model. However, producers of CO_2 in soils, microbial organisms, have a significant seasonal cycle (Lennon and Jones, 2011). These organisms usually have very high biomass and activity during growing season peaks with favourable conditions of temperature, moisture and substrate supply, and tend to be dormant under stressful conditions (Lennon and Jones, 2011; Stolpovsky et al., 2011; Wang et al.,

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2014; Wang et al., 2015). The seasonality of microbial biomass and activity, in addition to that of GPP and ST, may contribute to the seasonal variability of SR.

Additionally, lacking representation of macroinvertebrate and other forest floor and soil fauna in the ELMv0 may be another reason. There is a high density of earthworms at the MOFLUX site (Wenk et al., 2016). Earthworms can shred and redistribute soil C and change soil aggregation structure, which may alter soil C dynamics and CO_2 efflux to the atmosphere (Verhoef and Brussaard, 1990; Brussaard et al., 2007; Coleman, 2008). Like microbial organisms, earthworms usually have a significant seasonal cycle, showing high biomass and high activity during peak growing seasons and tending to be dormant during non-growing seasons (Wenk et al., 2016). However, a recent review suggests that current experimental evidence and conceptual understanding remains insufficient to support the development of explicit representation of fauna in ESMs (Grandy et al., 2016). Therefore, data collection focused on seasonal variations in fauna and microbial biomass and activity might enable further improvements in the representation of seasonal variation in SR.

Our analyses also showed that the modelled SR was not able to reach the observed peak in many years during the peak growing season, even when the modelled GPP exceeded the observation. In addition, the parameter modification increased GPP during both peak and non-growing seasons, resulting in an even greater overestimation of SR during non-growing seasons. These results suggest that simply increasing GPP may not be adequate to increase the seasonal variability of the simulated SR. A potential reason may be that the current model does not include root exudates. Root exudates are labile C substrates that are important for SR (Kelting et al., 1998; Kuzyakov, 2002; Sun et al., 2017). The root exudate rate is primarily dependent on root growth, showing a seasonal cycle in temperate forests (Kelting et al., 1998; Kuzyakov, 2002). Thus, including root exudates in the model may further increase the model simulated SR during the peak growing season without needing to increase GPP.

5 Conclusions

In this study, we used temporally extensive and spatially distributed site observations of SR to assess the capabilities of ELMv0. These results indicated that an improved representation of SWP within the model provided better simulations of annual SR. This underscores the need to calibrate SWP in ESMs for more accurate projections of coupled climate and biogeochemical cycles. Notwithstanding this improvement, however, the ELMv0 still overestimated SR during the non-growing season. It may be that inadequate model representation of the seasonality of fauna and microbial organisms could be explored as means to achieve better fit. Future incorporation of explicit microbial processes with relevant data collection activities may therefore enable improved model simulations.

Code availability. The code for ELMv0 is available at https://climatemodeling.science.energy.gov/projects/energy-exascale-earth-system-model

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Data availability. The data for this paper are available upon request to the corresponding author.

Competing interests. The authors declare that they have no conflict of interest.

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