Modeling perennial bioenergy crops in the E3SM land model (ELMv2)

Eva Sinha, Katherine V. Calvin, Ben Bond-Lamberty, Beth A. Drewniak, Dan M. Ricciuto, Khachik Sargsyan, Yanyan Cheng, Carl Bernacchi, Caitlin E. Moore

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Response to the reviewers

We thank the reviewers for their thoughtful and generally supportive assessment of our work. To address the reviewers' comments the following major additions/modifications were made to our analysis:

1. We re-performed the calibration to simultaneously calibrate all four quantity of interest.
2. We conducted model validation by reserving two years of carbon and energy flux measurement for validation and using the remainder for model calibration. We also used weekly LAI and annual harvest data for validation.
3. We used site level meteorological forcing data for model simulation instead of Global Soil Wetness Project Phase 3 (GSWP3) data used in the original submission.

In the following response we address the reviewers' concerns point by point. In addition, we have also added the version number of the E3SM land model to the title of our manuscript and have archived and made the source publicly available via Zenodo (`https://doi.org/10.5281/zenodo.5975834`).

Reviewer 1

Reviewer Point P 1.1 — General comments:

This study implements two perennial bioenergy crops miscanthus and switchgrass in the E3SM land model ELM. The revised phenology, carbon/nitrogen allocation, and biomass harvest parametrizations are based on the generic grass and annual crop functional types in CLM4.5 with the main distinction that the perennials are planted once and have repeated leaf onset, senescence and harvest cycle each year with a longer growing season than annuals. The manuscript focuses on sensitivity analysis and parameter optimization using an approach combining surrogate construction with polynomial regression and Bayesian calibration with MCMC. While the sensitivity analysis and calibration methods are novel, there are some issues that need to be clarified (which I list below as three questions). The manuscript can also be substaintly improved by an independent validation with data not used in the sensitivity analysis and calibration.

Reply: We thank the reviewer for recognizing the novelty of our work. We also agree with the reviewer on performing an independent validation that is now included in our analysis. Details of the model validation are discussed in comment P 1.3, P 1.7, and P 1.10.

Reviewer Point P 1.2 —

1. Are the constructed surrogate models each representing one quantity or variable of interest (QoI)?

2. From Table 2, I see that each parameter has different optimized values for different QoIs (GPP, ER, LE, H). For example, the parameter 'slatop' for Miscanthus used values 0.02, 0.06, 0.04, and 0.02 for estimating GPP, ER, LE, and H, respectively, in Fig. 3ACEG, right? Does it imply that the MCMC calibration was done for each QoI independently and that the ELM model or surrogate models were run multiple times using different parameter values to simulate the four QoIs in Fig. 3 separately?

My initial understanding is 'yes' to the above questions (correct me if I misunderstood and you can skip to 3, but please then explain what is the final value used for each parameter in Table 1 & 2 and how is it determined?)

This is the problem – Model calibration should lead to one decided value for each parameter for each bioenergy crop regardless of the QoI. A land surface model should have a determined set of parameter values to be used together to simulate all the carbon, water, and energy flux and state varaibles, including the QoIs here simultanuously, because they are interconnected. You can not use different (optimized) values for each parameter to simulate different target variables separately. Otherwise, you will have to conduct numerous runs for the large number of variables in ELM, which is not feasible for real applications. The calibrated results presented in Fig. 3 and Table 3 essentially come from the surrogate based posterior simulations for the respective QoIs, not from the ELM. Ideally, each parameter should be calibrated against all the observed variables (e.g., GPP, ER, LE, H) at the same time based on the average performance, so that it is applicable to other variables of interest such as LAI, carbon stocks, transpiration... in the same model.

Reply:

1. The surrogate models were developed for each day of year for all four QoIs (Figure A1 and A2). We have modified line 157 to state this more clearly.

2. Yes, in the original manuscript, calibration was performed independently for each QoI. The ELM surrogates were developed only once for each day of the year and for all four QoIs. However, MCMC calibration was performed separately for each QoI to find the optimal parameter value for the most influential parameters.

We agree that model calibration should result in a single set of parameter value for each quantity of interest (QoI) in order for these parameters to be utilized for future analysis. In the original submission we wanted to highlight how the most influential parameters vary based on the QoI, but we agree with the reviewer that having different set of parameters for various QoIs will increase the number of runs for the large number of ELM variables. We have, therefore, re-performed the calibration such that all four QoIs are simultaneously calibrated. We thank the reviewer for this comment that has improved the manuscript as well as provided a final set of optimized parameters for future analysis.

Reviewer Point P 1.3 —

1. The manuscript lacks an independent validation step to prove the model's generalizability and applicability for cross-location, regional, or global simulations. Validation usually entails applying the set of determined model parameters for each crop from calibration to one or more new sites to evaluate the model performance on all concerned variables or, if without new sites, at least reserving some observation data for evaluating some variables that are not used in the calibration. Although the 2000 ELM simulations were split to 1600 and 400 for training and testing the surrogates, it is not the same concept as validation. Fig. 3 is merely a calibration plot (and it is partial calibration/over-fitted to the input data for each individual QoI, thus lacking applicability to the ELM model as a whole). Therefore, the new model is not sufficiently validated yet.

Before the above questions are clarified, the current model development and evaluation are immature. If I did not misunderstood, the current model description and calibration are problematic and need to be revised. Essential steps to obtain a consistent set of parameter values for the ELM model (not for each QoI) and further validation of the model using independent data are needed.

Reply: This is a good point, and we now include model validation in the revised manuscript. For model validation, we reserved two years of observational data on carbon and energy fluxes and also utilized weekly leaf area index and annual harvest measurements. We used the optimized parameters obtained from model calibration to run a single model simulation for each crop and then compared the simulated output variables with observations for the validation years. This is described in more detail in sections 3.5, 4.5, and 5.0 of the revised manuscript.

Reviewer Point P 1.4 — Line 59: "ESM crop-models often use default global parameter values rather than crop- and region-specific values" – this is partly untrue. Take CLM4.5 for example, it uses crop-specific parameters for six major crop types, and it also considers regional differences for soy and maize by implementing tropical and subtropical cultivars for these two crops. It may be too challenging to use site-specific or region-specific parameters for a crop model in ESM if the objective of model development is for global applications.

Reply: We agree with the reviewer and have removed "crop-specific" from the text. However, region specific parameters are used in very few ESMs, and therefore we still mention that "region-specific values" values are "often" not used.

Reviewer Point P 1.5 — Lines 83-86: are these distinctive characteristics of perennial crops being reflected in the current model development for miscanthus and switchgrass?

Reply: The perennial bioenergy crops implemented in ELM capture the various phenological phases of these crops, which are distinct from annual crops. These crops also had fertilizer applied at a lower rate compared to maize (84 kgN/ha compared to 150 kgN/ha for maize).

Reviewer Point P 1.6 — Section 2.1: The described phenology is very similar to annual crop phenology, except that annuals are planted every year, but perennials are planted once and have repeated leaf onset, growth, senescence and harvest cycle each year. The major difference of the two perennial crops from the generic grass is their longer growing season and "planting once", while the phenological cycles are essentially the same as annual grass/crop in CLM4.5/ELM. It seems the Cheng et al. 2020 study also used this strategy to simulate miscanthus and switchgrass (please verify the statement in Line 291-294).

Reply: The perennial bioenergy crops modeled in this study differ from their depiction as annual crops in CLM by Cheng et al. [2020]. The major difference is that in this study the perennial bioenergy crops have only three phenological phases—crop emergence, leaf onset, and leaf senescence—while Cheng et al. [2020] model bioenergy crops as annual crops with four distinct phenological phases that include planting, leaf emergence, grain fill, and harvest. Second, the requirements for the start of various phenological stages is different between this study and Cheng et al. [2020]. In this study the perennial bioenergy plant emergence occurs when temperature thresholds are met between the minimum and maximum planting days. This is slightly different than perennial crop emergence in Cheng et al. [2020] that is based on temperature and growing degree day (GDD) criteria. In this study the perennial bioenergy crop leaf emergence occurs when the accumulated GDD exceeds the crop-specific minimum GDD requirement, while in Cheng et al. [2020] the annual crop leaf emergence occurs when a fraction of the GDD required for maturity is reached. Lastly, in this study leaf senescence for the perennial bioenergy crop occurs when the temperature and leaf age criteria are met, while in Cheng et al. [2020] plant reaches senescence when GDD maturity is reached. These differences result in a better capturing of the various phenological phases of the bioenergy crops in this study than in Cheng et al. [2020].

We have revised text in lines 344–349 in the Discussion section to clearly state the differences between the two studies.

Reviewer Point P 1.7 — Section 3.3: Isn't there LAI and/or biomass harvest data for the two crops? It would be beneficial to have harvest data for validation of the model, given that this is the key output of interest for bioenergy crops.

Reply: We thank the reviewer for this suggestion. Yes, weekly LAI and annual harvest data are available for the two crops, and we have included model validation using these two output variables.

Reviewer Point P 1.8 — Line 208: the seasonal dynamics of H is poorly simulated by the ensemble. It will be good to see more explanation why the observed trough of H in the summer season (May-Aug) is not captured by the model.

Reply: The majority of ensemble members overpredict H during the growing season. We have added this clarification in the revised manuscript and added an explanation on the possible cause of this discrepancy (lines 231–235).

Reviewer Point P 1.9 — Lines 231-232: this could be mentioned earlier in the methods section when describing the construction of surrogates.

Reply: Lines 231–232 in the original manuscript describe the most influential parameters identified during the global sensitivity analysis. We are guessing that the reviewer's suggestion was to move lines **213–214** (*"We utilized 1600 of the 2000 ELM simulations for developing the surrogates using PC surrogate form and 400 simulations for testing the accuracy of the surrogates"*) to the methods section. We have moved this line to Section 3.1 on surrogate construction.

Reviewer Point P 1.10 — Section 4.4, Lines 236-239: From here I realize that the authors calibrated the parameters for the four QoIs separately and obtained different optimized parameter values for the different QoIs in Table 2. Thus, I asked the above main questions. Only if the authors have determined a final set of parameter values for each crop type (not for each QoI) and validate the whole model using this parameter set against various observations of (e.g., LAI, carbon stocks, harvested biomass, etc.) in addition to the variables used for calibration (GPP, ER, LE, H), can we trust that the new model is fully developed and validated for real world applications.

Reply: We agree with the reviewer's comment regarding providing a final set of parameter values and validating the model. We have revised the manuscript to simultaneously calibrate all four QoIs, resulting in a single set of optimized parameter values (see P 1.2 for more details). We also conducted model validation by utilizing two years or carbon and energy flux measurements and LAI and harvest measurements for model validation (see P 1.3 for more details).

Reviewer Point P 1.11 — Lines 243-245: these less reliable parameters are the most sensitive ones – What is the implication for the model accuracy? This needs to be discussed.

Reply: We have added explanation on the implications of these less reliable parameters on model accuracy in lines 269–271 of the revised manuscript.

Reviewer Point P 1.12 — Lines 262-263: this same reason should also lead to decreased H during the summer season, which is not well captured by the model.

Reply: Agreed. We have made modifications to line 288–289 of the revised manuscript to clarify this.

Reviewer Point P 1.13 — Line 264: the diurnal mismatch is likely related to plant hydraulics and soil hydraulics.

Reply: We thank the reviewer for this suggestion, however, since we did not investigate the cause of diurnal difference between observations and simulations we have not added this probable cause in the manuscript.

Reviewer Point P 1.14 — Line 265: not really captured the seasonality, esp. for Sep. and Oct. as shown in Fig. 3H

Reply: For switchgrass, the simulations capture the seasonality but not the observed magnitude during the summer months, while for miscanthus neither seasonality nor magnitude is captured by the model. We have described this more clearly in the revised manuscript (lines 291–295).

Reviewer Point P 1.15 — Section 5: The Discussion is focused on sensitivity analysis and calibrated parameters. While they are an important step of model development, the discussion could devote more to validation and comparison of model performance with reference to observation or the literature, and the implications for model application in potential research fields. For example, why the model failed to capture the seasonality of sensible heat? And can the model correctly simulate harvested biomass or soil carbon pools (which are important consideration for bioenergy crops)? Even if there are no direct observations at the study site, there may be published data or related information in the ecology or agricultural literature.

Reply: We have added a new paragraph in the Discussion section that focuses on model validation.

Reviewer Point P 1.16 — The manuscript can also be improved if the authors clearly list the limitations and uncertainties of the current model.

Reply: The last paragraph in the Discussion section now lists the limitations of current ELM-crop model.

Reviewer Point P 1.17 — Line 300: Given the high sensitivity of the model to this parameter, even if the optimized range of slatop matches observed range, a single value of slatop should be decided for each crop functional type in order to be used in cross-site or regional simulations. Please see earlier comments about this issue.

Reply: We agree that a single value of the parameter should be identified. In the revised manuscript, when we performed combined calibration of all four QoIs, `slatop` was not selected among the five most influential parameters and was therefore not optimized. As a result, the default value of this parameter was used in model validation. We have removed the paragraph in the original Discussion section that compared optimized `slatop` value with observations collected at various sites.

Reviewer Point P 1.18 — Lines 325-326: Why water budgets but not carbon budgets and harvests? Carbon is the major concern for bioenergy crops. Again, calibrating a land surface model using spatially varying site data would lead to spatially varying parameter values, which may work for those specific sites used for calibration, but cannot guarantee their applicability to other places or to regional and global simulations. That's why I commented that the current study lacks an independent validation using the calibrated and determined parameter set against different datasets and/or different variables of interest.

Reply: We wanted to imply that apart from calibrating the model outputs to carbon and energy budget, future studies can also calibrate to water budget that was not included in this study. However, lines 325–326 in the original manuscript did not convey this clearly. We have revised the sentence to better convey the message and also suggested validation using measurement at other sites to test model applicability.

Reviewer Point P 1.19 — Figure 1: it would be helpful to add the ensemble mean of model simulations, not just the range.

Reply: Ensemble mean has been added in Figure 1.

Reviewer Point P 1.20 — Table 2: explain what the dash "-" means.

Reply: The dash in Table 2 of the original manuscript implied that the parameter was not the most influential parameter for a particular QoI and therefore the default value for this parameter was sufficient for the particular QoI. However, in the revised manuscript, when we simultaneously calibrated all four QoIs, the five most influential parameters were the same for both miscanthus and switchgrass, and thus no dashes are used in Table 2.

Reviewer 2

Reviewer Point P 2.1 — The authors attempted to improve the representation of perennial bioenergy crops in ELM and identified the sensitive parameters to evaluate the performance of the newly developed module - ELM-crop. I have some concerns. First, there are not many improvements that have been made in the ELM-crop. The authored adopted a lot of processes and parameters from ELMv1 or CLM4.5, described in section 2. I am not sure what is the major contribution that the authors have made to develop the ELM-crop module. Second, since the authors were modeling crops, fertilization should be considered. How does the ELM-crop deal with fertilization (nitrogen input, plant uptake, nitrogen emissions, and leaching/runoff)? I did not see any detailed description on this, nor about the input data sets. Third, the authors only calibrate the newly developed model at one site. How does the model perform at other sites? Fourth, although the authors spent a lot of energy on parameter optimization, I do not think they were necessary enough to improve the ELM-crop module that they developed. Moreover, the comparison of daily GPP shown in Fig. 1 looks far from good for Miscanthus.

Reply:

1. The main contribution of this work was adding perennial crop modeling in ELM and parameterizing the model for two bioenergy crops; miscanthus and switchgrass. Perennial crops did not exist in ELM prior to our study and have phenological stages distinct from annual crops. The different phenological stages of perennial crops were included in ELM as part of this study and are described in Section 2.1. The carbon and nitrogen allocation scheme and harvest for perennial crops do have many similarities to that of annual crops.

2. ELM-crop model does account for nitrogen input, uptake by plants, nitrogen leaching, and nitrogen emissions:

   (a) Fertilization is considered in this study and is applied to both bioenergy crops after crop emergence at a rate of 84 kgN/h over a period of 20 days to maximize nitrogen utilization by plants and minimize nitrogen loss through denitrification. We now describe the fertilizer application approach in lines 90–91 of the revised manuscript.

   (b) In addition to fertilizer application, for the annual crops the ELM-crop module also accounts for nitrogen retranslocation from leaves and stem to the organs during grain fill stage and for nitrogen fixation by soybean crop [Drewniak et al., 2015]. Additionally, ELM also accounts for loss of nitrogen to the atmosphere and nitrogen leaching from land [Burrows et al., 2020].

   (c) The input data set is described in Section 3.3.

3. An independent validation of the model is now included in our analysis. Due to a lack of carbon and energy flux observations for other sites, we used observational data from the same study site (but different years) for both model validation and calibration. Details of the model validation are discussed in comment P 1.3, P 1.7, and P 1.10.

4. We respectfully disagree with the reviewer' comment regarding the added value of parameter optimization. Figure 1 displays the large ensemble spread of various QoIs when the model run was performed using randomly varying value of the 20 input parameters. The GSA analysis identified the most influential parameters while the calibration identified the optimal value of

these parameters. The calibrated GPP based on the optimal parameter values (Figure 3A and 3B) captures various phases of the plant growth and magnitude accurately, except for slightly underpredicing peak GPP.

Reviewer Point P 2.2 — Line 17: Here, does "agriculture" include pasture? Or do you mean "cropland only"?

Reply: The term agriculture in Line 17 was referring to croplands only and did not include the land used for grazing. However, we agree with the reviewer that agriculture can be interpreted as sum of cropland and grazing land. Therefore, we have replaced "agriculture" with "cropland" in Line 17.

Reviewer Point P 2.3 — Line 46: Provide the full name of "ISAM". Also, in lines 49 and 52 for "ORCHIDEE" and "JULES".

Reply: Addressed.

Reviewer Point P 2.4 — Lines 54-55: This sentence seems out of place. The authors should introduce the importance of parametrization optimization when they describe all improvements made in previous land models. Then, they can conclude this. I think it is necessary to add this description.

Reply: We have moved the line describing the importance of parameter optimization earlier in the paragraph (lines 46–47).

Reviewer Point P 2.5 — Lines 71-76: This paragraph fails to convey the objectives of this study. It is necessary to describe what the authors have done in order like (1) the improvements of perennial crops in ELM; (2) the calibration scheme; (3) validation if the authors have done; and (4) the key implication or the regional application of the newly developed module at the regional scale.

Reply: We have made modifications in the last paragraph of the Introduction to more clearly state the objectives of our study. Perennial crop modeling did not exist in ELM before this study was conducted and thus its addition in ELM was one of the main objective of this study.

Reviewer Point P 2.6 — Lines 78-79: The authors should add one or two sentences to describe this. Also, at least one sentence for explaining the major difference between ELMv1 and CLM4.5.

Reply: We have added major differences between ELM and CLM4.5 in the text.

Reviewer Point P 2.7 — Lines 85-86: ELMv1 has not (or partially?) considered nutrient input, allocation, and limitation, right? Did you improve all these processes in the newly developed version?

Reply: ELM-crop model does account for nitrogen input and its allocation among the various plant components during the growth phase [Drewniak et al., 2015] (also see P 2.1).

Reviewer Point P 2.8 — Section 2.2: I am confused. I think carbon and nitrogen allocation in perennial crops are different from the annual crops, but in this section, it seems that the authors just adopt these processes from the annual crops in ELM. So, what is the authors' contribution?

Reply: In this study, we implemented perennial crops that have phenological phases that are distinct from annual crops. The three phases of perennial crops – crop emergence, leaf onset, and leaf senescence – all have requirements different from annual crops. Additionally, perennial crops modeled here do not have grain fill phases that is considered for annual crops in ELM. In this study, the carbon/nitrogen (CN) allocation for perennial crops between leaf emergence and leaf senescence is kept similar to the CN allocation for annual crops between leaf emergence and the start of the grain fill stage.

Reviewer Point P 2.9 — Section 2.3: What do you mean "a single time step after occurrence of the leaf senescence."? Any range for the number "70% of the available C and N contributes..."?

Reply: For perennial crops leaf senescence occurs when temperature and leaf age criteria are met (Eq. 6 and 7). Harvest occurs, as soon as the leaf senescence criteria are met. During harvest 95% of the aboveground biomass in the form of carbon and nitrogen stored in leaves and live stems is converted to biofuel. We have modified section 2.3 to describe the harvest process more clearly.

Reviewer Point P 2.10 — Line 135 and 146: Give the full of QoIs in the first place.

Reply: Addressed.

Reviewer Point P 2.11 — Section 3.1: It is necessary to describe your input data sets such as meteorological conditions, nitrogen fertilization, soil property, etc. To my knowledge, the authors should drive the ELM-crop with all inputs from the selected site at the University of Illinois Urbana-Champaign (UIUC), right? In line 173, the authors mentioned the eddy covariance flux towers. I think it is necessary to give the names of these flux towers. One more question about the calibration: The authors only described the calibration. Do they have any other site-level data for model validation?

Reply:

1. The site data including meteorological conditions, soil type, planting dates, fertilize application rate, and harvest time were described in the section 3.3 of the original manuscript (lines 165–173).
2. The model estimates the crop emergence and harvest dates based on when temperature and growing degree days, criterias are met (Section 2.1). In the revised manuscript we re-ran the model simulations by utilizing site specific meteorological data instead of Global Soil Wetness Project Phase 3 (GSWP3) data used in the original submission.
3. We are not aware of the name of the eddy covariance flux towers, however, we have added site names in line 179 of the revised manuscript.
4. In the revised manuscript we have included model validation (discussed in comments P 1.3, P 1.7, and P 1.10).

Reviewer Point P 2.12 — Fig. 3a: The peaks of modeled GPP shifted compared to the observation for Miscanthus. Can you explain?

Reply: In the revised manuscript calibration results were modified slightly compared to the original submission because of site specific meteorological data being utilized instead of GSWP3 and because all four QoIs were simultaneously calibrated. The calibration results, however, are similar to those described in the original submission. The calibrated GPP captures the timing of peak GPP and the sharp increase before peak GPP, but slightly underestimates the magnitude of peak GPP. This is explained in Section 4.4, and is expected, since all four QoIs are now simultaneously calibrated, resulting in less than optimum calibration for individual QoIs.

References

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