Response to reviewer #1

General comments

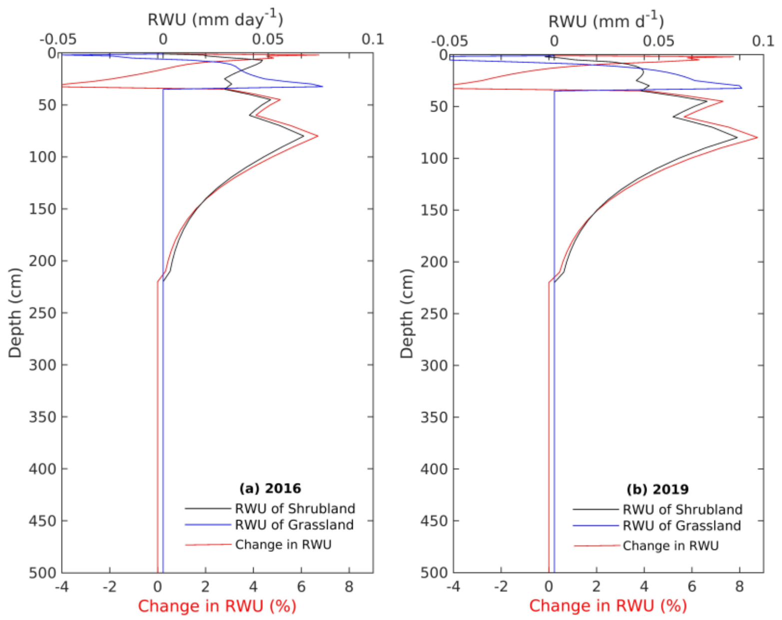
This study applied the STEMMUS-SCOPE model to a typical revegetation plot which consists of shrubs and grass, to simulate the impact of revegetated shrubs on surface fluxes (latent heat flux, sensible heat flux, and GPP) and soil moisture. While the manuscript describes a lot about the comparison between the two scenarios, I more focus on the model and the model configuration, and how this study can contribute to model development or deepen our understanding the effect of revegetated shrubs. In general, I think this part of work is weak.

Thanks for your thorough review and detailed comments on our article. Indeed, the model configuration is the key to represent the fluxes in mixed vegetated areas. In this study, we employed two sets of parametrizations and ran the model separately for two land covers. The accuracy of the composited fluxes demonstrated the feasibility of distinguishing the LAI using HANTS and fractional vegetation coverage to separate the two land covers *(see Section 4. Performance of model calibration in Supplement)*. With this understanding, our goal is to achieve parallel computation of the two land covers in the next model version, with more consideration on interaction of root growth and root water uptake. Below, we address the specific comments related to the model configuration and interpretation of results.

Specific comments

1. *Line 29, in the introduction section, the scientific question is not clear. Generally, the authors thought root water uptake is a critical process in the modeling, and the dynamic root length density for estimating root water uptake is necessary. However, no contents about the root water uptake were presented in this study. What is the impact of dynamic root length density? What is the performance of root water uptake simulation? This is the major limitation of this study.*

Response 1: Thank you for the insightful suggestions, which will be addressed in the revised manuscript. We did calculate the root zone water storage in 0-200 cm depth (Eq. S15 in the Supplement). And we found that the replacement of shrubs decreased root zone water storage in 2016 (-27%) and 2019 (-11%), respectively. It is a great idea to show the simulation of root water uptake (see figure on the right side), where we compared the root water uptake (RWU) of shrubs and grasses in 2016 and 2019, respectively.



In general, the RWU of grasses (shrubs) increased from the surface layer and then decreased to zero at 30 cm (200 cm) depth. This pattern is highly related to their maximum rooting depths, which were predefined parameters in our model. Moreover, our model successfully captured hydraulic redistribution, as indicated by negative RWU values in the relatively shallow root zone (Kennedy et al., 2019; Wang et al., 2021). The negative RWU values resulted from the higher root water potential (in absolute value) compared to the soil water potential when the surface was too dry in the study area.

To quantify the change in RWU, we used the RWU of grasses as the control reference, then the Changes in RWU (red line) was calculated by $(RWU\ of\ shrub - RWU\ of\ grass)\ /\ RWU\ of\ grass$. When comparing the Changes in RWU, we noticed that the replacement by shrubs reduced RWU at the 0-30 cm depth but increased RWU at the 30-200 cm depth. This observation aligns with the pre-defined root distribution of shrubs and grasses. However, it is important to note that we currently lack observed data to validate the performance of any root simulation in our study.

Refer to the Comments 7, 8 and 12, we will include the root parameters in the sensitivity analysis and optimize them accordingly. Besides, we will analyze the effects of revegetation on root water uptake in a more detailed manner in the revised manuscript. Besides, we will include the equations of RWU and root growth simulation in the revised supplement.

2. *Line 92. The quality control of flux data was missing. Moreover, how did you calculate GPP?*

Response 2: Thank you for your attentive review. If necessary, we will include this section in the supplement. The steps to calculate GPP from the raw EC flux are as follows:

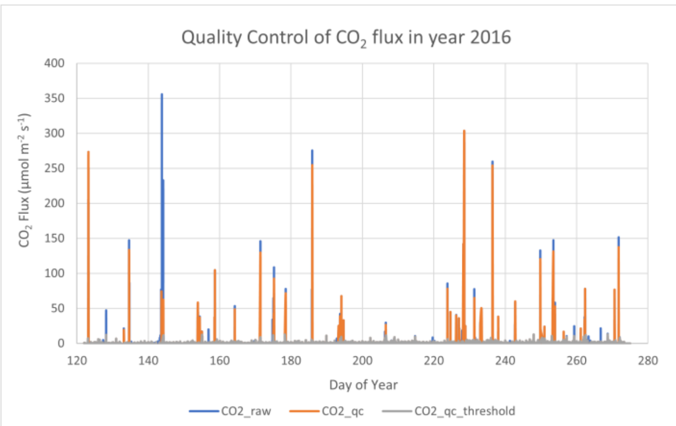
(1) Pre-processing: The raw flux data was first proceeded with EddyPro software.

(2) Processing: Quality control was conducted. If the value fall in the range as following, it's the invalid value that was set as NA, otherwise the original value was kept.

- qc = 2
- NEE ≤ -15 and NEE ≥ 15;
- LE ≤ -20 and LE ≥ 550;
- H ≤ -60 and H ≥ 400;

Take the CO_2 flux as an example,

Timestep (0.5 hour)	Raw data	qc = 0 or 1	qc = 0 or 1 & -15 ≤ NEE ≤ 15
2016	7344	6602	6496
2017	3314	2342	2322
2018	4368	3986	3906
2019	7344	5297	5159



(3) Post-processing: Following quality control, NEE is partitioned into GPP using the REddyProc package in R, which involves u* filtering, flux partitioning, and gap-filling steps. Solar radiation (Rg), air temperature (Tair), relative humidity (Rh), and vapor pressure deficit (VPD) were used in this process. The partitioning principle is based on two relationships: (1) at night, Ecosystem Respiration = Net Ecosystem Productivity = - Net Ecosystem Exchange because Gross Primary Productivity is zero at night; (2) Gross Primary Productivity = Net Ecosystem Productivity - Ecosystem Respiration.

3. *Line 125. How did you determine the contributions for shrubland and grassland?*

Response 3: The contributions for shrubland and grassland are determined by their fractional vegetation cover. Based on a high-resolution image taken by unmanned aerial vehicle (Fig. S2), the Supervised Classification Method in ERDAS 2020 was employed to determine the fractional cover of shrubs (35 %), grasses (25 %) and bare soil (40 %). Since STEMMUS-SCOPE considers the soil-root-canopy continuum, we implicitly included the bare soil in either shrub grids (58.33 %) or grass grid (41.67 %). The uncertainties of estimating the fractional cover based on limited image were indicated in Line 370.

4. *Line 136, can 500 m-MODIS LAI represent the 30 m fenced area?*

Response 4: Indeed, it might be not representative especially for the sparse and mixed vegetated area (Fensholt et al., 2004; Fensholt and Sandholt, 2005). That's why we tried to reconstruct the MODIS LAI using field observations and relevant literature values, in order to ensure this critical input as representative as possible. We corrected the MODIS LAI by the correlation ratio that was estimated based on relationship between MODIS LAI and field measurement in 2022, and lastly compared the corrected values in 2016-2019 with literature values (Line 150, Figure 2). However, the MODIS LAI was used as reference because of its availability and relatively high temporal resolution.

5. *Line 139-140, how did you determine the values of 2.33 and 1/4?*

Response 5: Sorry if this was unclear in the manuscript and this will be clarified in the revised version. First, The MODIS 4-day LAI data during 2016-2019 was smoothed by the Harmonic Analysis of Time Series (HANTS) algorithm (i.e., LAI_{HANTS}). Second, the linear relationships were determined between LAI_{HANTS_shrub} and two observed LAI for shrub (LAI_{actual_shrub}) in 2022. The correlation ratio ($ratio = \frac{LAI_{actual\_shrub}}{LAI_{HANT\_shrub}}$) were determined as 1.92 and 2.73 for DOY 160.5 and DOY 168.5, respectively. The final correction ratio applied in LAI_{HANTS_shrub} ends with value of 2.33, which is the average of 1.92 and 2.73. For detailed calculations of LAI_{actual_shrub}, please refer to Table S4 in the Supplement.

For the LAI of grasses (LAI_{grass}), it was estimated as 1/4 of that of the shrubs (LAI_{shrub}) based on the following constraints (Line 140 – Line 145):

i. $LAI_{shrub}(i) \approx 4\ LAI_{grass}(i)$ (Dan et al., 2020)

ii. $LAI_{grass}(i)$ should follow the temporal pattern of $LAI_{MODIS}(i)$ and it was ~0.5 $m^2\ m^{-2}$ (Yang et al., 2019; Dan, 2020)

iii. $f_{shrub} * LAI_{shrub}(i) + f_{grass} * LAI_{grass}(i) + f_{baresoil} * LAI_{baresoil} = LAI_{MODIS}(i)$

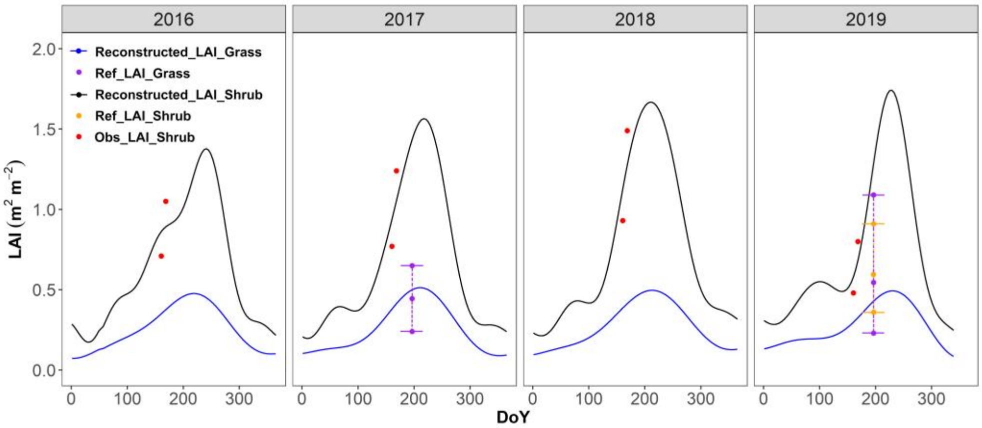
iv. $f_{shrub} + f_{grass} + f_{baresoil} = 1$

v. $LAI_{baresoil} = 0$

where f_{shrub}, f_{grass} and $f_{baresoil}$ are the fractional cover of shrubs (35%), grasses (25%) and bare soil (40%), respectively.

6. *Line 151, what is the difference between red and yellow dots?*

Response 6:



Line 150 Figure 1. Reconstructed LAI of shrubland and grassland from 2016 to 2019.

The yellow dots and purple dots are reference values from literature while the red dots are the actual observed value of shrub. In Figure 2 (Line 150), the yellow dots and dotted lines (Ref_LAI_Shrub) represent the ranges of measured LAI of the nearby shrublands from the reference of Dan, 2020. The red dots (Obs_LAI_Shrub) are the actual LAI of shrubs on DOY 160.5 and DOY 168.5, where we did not have real measurement, but we calculated them based on the correlation ratio derived in 2022 (Table S4 in the Supplement).

7. *Line 176, why were root-related parameters not identified as influential parameters? This is the main focus of your study.*

Response 7: Thank you for bringing up this important point! In STEMMUS-SCOPE, the maximum rooting depth, fitted extinction coefficient, and root length density are the primary rooting parameters in determining root distribution, root growth, and root water uptake (Jackson et al., 1997; Wang et al., 2021). In the revised version, we will incorporate these parameters into the sensitivity analysis.

8. *Line 216, how did the authors optimize the parameters (best-fit trail in Line 196)? How to avoid the equifinality for the parameters of shrub and grass?*

Response 8: During the sensitivity analysis, 160 sets of parameters for shrubland were generated and while a fixed parametrization was used in grassland simulation. As a result, the shrubland simulation generated 160 sets of fluxes, which were aggregated with the fluxes from the grassland simulation. By comparing the 160 sets of aggregated fluxes with the observed fluxes, we calculated the R^2 and RMSE for each flux in each trail. At last, an objective function, the normalized root mean square errors $RMSEn = \frac{RMSE_{SWC}}{\overline{Obs}_{SWC}} + \frac{RMSE_{LE}}{\overline{Obs}_{LE}} + \frac{RMSE_{GPP}}{\overline{Obs}_{GPP}}$ was calculated for each trail, where $\overline{Obs}_{SWC/LE/GPP}$ is the average values of observed SWC, LE and GPP throughout the investigation period, respectively. The best-fit trail (i.e., the optimized parametrization for shrubland) is the trail with minimal $RMSEn$.

The equifinality for the 160 sets of shrub parameters might be an issue, especially in such a non-linear system with many physical processes. We mitigated the equifinality problem by considering two aspects: (1) For the sensitivity analysis method, we used the Morris method - a global sensitivity analysis method. On the one hand, the Morris method samples parameter values from a given interval in a large parameter space (i.e., 16^7 in our case). This systematic sampling approach ensures a broad exploration of the parameter space, which can help identify the model's sensitivity to different regions. On the other hand, except for ranking the influence of parameters based on elementary effect, the Morris method also quantifies interactions between parameters, which helps understand how parameters jointly affect the model output; (2) For the sensitivity analysis result, the use of objective function $RMSEn$ in requiring RMSE in SWC, LE and GPP can help avoid this problem. More samplings and analysis can be done but is beyond the focus of this study.

9. *Line 218, does it mean Vcmax of shrub and grass is the same (120)? Why?*

Response 9: Yes, in this work, we assume the maximum carboxylation rate (Vcmax) is the same for both shrubs and grasses. In light of the reference values from studies involving similar shrub species, Vcmax = 120 for shrub was determined (Wang et al., 2017). For the grassland, the default value for C3 grassland is 80 in SCOPE model and we did not find any reference value for similar species or in similar study area. We assume the same Vcmax for grass as shrub in order to maintain consistency for the species grown in the same study area, regarding their adaptability to the arid region. Besides, the grassland simulation serves as a reference scenario pre-revegetation. The Vcmax variation in the grassland simulation doesn't impact the primary goal: comparing grassland and shrub-grassland scenarios. But indeed, a more representative Vcmax could improve the physical interpretability when comparing two scenarios.

10. *Line 237, the sensors were installed under the grassland, but the simulated soil water content is the average of shrub, grass, and bare soil. So, direct compassion of them may have a large bias.*

Response 10: We fully agree on this and will point out the bias in the discussion in a more detailed manner. Since the soil water content is a state variable, which is not reasonable to aggregate/average from shrub, grasses and bare soil simulation in current modelling scheme. Therefore, we ended up with comparing the observed soil moisture with the simulated soil moisture from the grassland simulation.

11. *Line 373, why did not the author attempt to modify the model to simulate evaporation from the bare soil?*

Response 11: We did not simulate the evaporation or soil moisture from bare soil individually because STEMMUS-SCOPE considers the soil-root-canopy continuum, and quantifies the amount of energy received and water evaporated based on the leaf area index, gap fraction and leaf inclination. The key idea of this study is to compare the difference in the fluxes between grassland and shrubs-grassland scenario, in order to represent the effects of planting shrubs. Hence, we thought the current modelling scheme adequately represents fluxes in a mixed vegetated area. However, it's worth noting that the STEMMUS model itself can simulate evaporation from bare soil effectively (Zeng et al., 2011), while STEMMUS-SCOPE is more adaptable for vegetated areas (LAI > 0). To address this issue, future model improvements will aim to allow the option of switching on/off the vegetation module as needed.

12. *Line 403. Why cannot the model capture the wet deep soil layer? Is it related to root water uptake? More analysis and simulation should be performed.*

Response 12: Sorry if this was unclear in the manuscript. According to the observed dry surface (i.e., low SWC at 10 cm) and a higher observed LE and GPP compared to the simulations, we assumed that the shrubs could switch their root water uptake strategy by either accessing the deep soil water and/or accessing water by lateral roots. If the former assumption is met, our model does not have this option for the plant to switch RWU under specified condition but only simulate the root length growth and RWU by root parameters mentioned in **Response 7.** For the latter assumption of lateral roots, our model is a 1-D vertical model therefore we overlook this process, which is an important survival strategy of shrubs in the study area.

For the RWU simulation, the uncertainties were raised from (1) the setting of the initial soil profile. As shown in the (user-defined) initial conditions (Table S2), the soil moisture under 10 cm was estimated without support from observations during 2016-2019. In the STEMMUS-SCOPE, the initial SWC profile not only determines the pattern of soil water storage but also indicates the pattern of root water uptake in the soil column. That's why we mentioned *"the model might not capture the wet deep soil layer"*; (2) The uncertainties in reconstructed LAI; (3) The uncertainties in estimated Vcmax and root parameters.

However, these are just plausible assumptions because of the lack of observed data from underground. Future analysis will be conducted by investigating the root parameters and modules, to gain more insights and clarifications in the revised manuscript.

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