We thank the editor for the time and effort in facilitating the reviewing process and the reviewers for their constructive comments. Please see our point by point response as follows. The reviewers' comments are in black fonts indexed by numbers. Our response is in blue fonts and red fonts are the updates in the manuscript.

Referee #1

General Comment: The manuscript by Yu et al. presents a study assessing the role of model complexity of soil physics processes on simulation of vegetation dynamics for a Tibetan meadow site. Three different model versions of the T&C model, with a gradual increase in the complexity of the freezing-thawing treatment, are compared: (1) the original T&C model, lacking soil freezing processes; (2) a modification of T&C in which an ice fraction and freezing/thawing are accounted for; and (3) a coupling of T&C to the soil physics model STEMMUS. The model versions are parameterized and driven with data from a Tibetan meadow site to evaluate their performance. Differences between results with the three versions of the model are small for most variables, generally smaller than the model-to-data difference, and the simulated differences are confined to parts of the year where freezing dynamics are likely to play a role. The analysis would benefit from a focus on specific periods of the year where differences arise.

This manuscript is potentially of interest to the readers of The Cryosphere and contains an interesting discussion on the role of freezing-thawing for ecosystem processes in high latitude and high altitude environments, and the importance of model complexity in ecohydrological models. However, in its current form, it contains many inaccuracies in the presentation of the results and ambiguity in the presentation of the model versions, simulation setup and the results, which make it hard to judge the models' qualities. I cannot recommend publication given the current state of the manuscript, but with substantial modifications in the texts and the presentation of the results, I expect that this could become suitable for publication in The Cryosphere.

Response: Thanks a lot for your insightful comments. We rearranged the manuscript structure to make it more readable. The experimental site (and its multi-component measurements) was introduced in Section 2. The STEMMUS and T&C models (and their coupling), as well as numerical experiment designs (and key governing equations) were introduced in Section 3. Equations for different model versions were clearly presented in Sect. 3.1-3.4. Section 4 detailed results and discussions on the role of different vadose zone physics in the ecohydrological response to freeze-thaw cycles. Section 5 summarized the potential influential pathways of different vadose zone physics, and the study was concluded in Section 6. We added Table 1 to clarify the difference among three models (see Sect. 3.5). The constitutive equations regarding unfrozen water content, ice effect on hydraulic conductivity, the temperature dependence of water flow, water vapor density were given in Supplement S1. We added figures in supplement materials to present the surface energy fluxes simulations during the non-frozen and frozen period, respectively. The relevant text

was added to the manuscript and supplement Section S2 to explain the differences among the three models. We added Figure 1 to illustrate the geophysical location of Maqu soil moisture and soil temperature (SMST) monitoring network, indicating the central experimental site where our data were collected. Thus the figure numbers in the revised manuscript were all updated correspondingly.

1. The introduction discusses model improvement in very broad terms, but it does not give a rationale for focusing on soil freezing processes specifically in this study. I would suggest using the introduction instead for a more in-depth discussion of the role of freezing-thawing processes for ecosystem dynamics and the limitations of current models in representing these.

Response: Thank you very much. We updated the introduction part adding more focus on the role of the freezing-thawing process for ecosystem dynamics and we discussed the limitation of current models in representing these processes.

2. - Title: The current title is grammatically incorrect. I would suggest removing the question mark at the end of the sentence. Alternatively, "affects" can be replaced by "does affect" (i.e., How does vadose zone mass and energy transfer physics affect the : : :")

Response: Thanks a lot. We removed the question mark and rephrased the title as "On the Role of Vadose Zone Physics in the Ecohydrological Response of a Tibetan Meadow to Freeze-Thaw Cycles"

3. – Introduction: The first part of the introduction (L. 33-43) is not very informative for the problem assessed in this manuscript: It describes in general terms the gradual improvements that have been undertaken in many different types of models, without a clear focus on the research

Response: Thanks a lot for your insightful comments. We modified the first part of the introduction and focused on the response of ecosystem dynamics in cold regions, and on the ongoing modeling efforts with consideration of vegetation and freeze/thaw process. Then we further stressed the relevance to consider the coupling water and heat physics in cold regions.

Changes in the manuscript: "Recent climatic changes have accelerated the dynamics of frozen soils in cold regions, as for instance favoring permafrost thawing and degradation (Cheng and Wu, 2007; Hinzman et al., 2013; Peng et al., 2017; Yao et al., 2019; Zhao et al., 2019). In consequence of these changes, vegetation cover and phenology, land surface water and energy balances, subsurface soil hydrothermal regimes, water flow pathways were reported to be affected (Campbell and Laudon, 2019; Gao et al., 2018; Schuur et al., 2015; Walvoord and Kurylyk, 2016; Wang et al., 2012). Understanding how ecosystem interacts with changing environmental conditions is a crucial yet challenging problem of Earth system research for high latitude/altitude regions and deserves further attention.

Land surface models, terrestrial biosphere models, ecohydrology models, and hydrological models have been widely utilized to enhance our knowledge in terms of land surface processes, ecohydrological processes

(Fatichi et al., 2016a;Fisher et al., 2014), and freezing/thawing process (Cuntz and Haverd, 2018;Druel et al., 2019;Ekici et al., 2014;Wang and Yang, 2018;Wang et al., 2017b). For instance, Zhuang et al. (2001) incorporated a permafrost model into a large scale ecosystem model to investigate soil thermal temporal dynamics. Zhang et al. (2018) investigated the long term high-latitude Arctic tundra ecosystem response to the interannual variations of climate with the process based CoupModel. The LPJ-WHy model, with consideration of permafrost dynamics and peatland, was used to analyze land surface processes by Wania et al. (2009). Lyu and Zhuang (2018) coupled a soil thermal model with the Terrestrial Ecosystem Model (TEM) to explore snowpack effects on soil thermal and carbon dynamics of the Arctic ecosystem under different climate scenarios."

4. - L. 16: consider inserting "those relevant for" after "parameterizations"

Response: We rephrased the text here. see Line 17.

5. - L. 23: "The difference among various complexity: : :": This sentence is unclear; the meaning of "among various complexity" needs to be specified.

Response: We modified this sentence as "The physical representation is increased from using T&C without, and with explicit consideration of ice effect, to T&C coupling with STEMMUS enabling the simultaneous mass and energy transfer in the soil system (liquid, vapor, ice)."

6. - L. 26: Remove comma; also, I think that "in ecosystem functioning" should read "for ecosystem functioning".

Response: We have removed the comma and replaced "in ecosystem functioning" with "for ecosystem functioning". See Line 27.

7. - L. 58: "there are divergences". Please explain these divergences.

Response: We explain the divergences in the context as "In response to climate warming, the degradation of frozen ground can positively affect the vegetation growth in Tibetan Plateau mountainous region (Qin et al., 2016), but it can also lead to degradation of grasslands (Cheng and Wu, 2007), depending on soil hydrothermal regimes and climate conditions (Qin et al., 2016; Wang et al., 2016). " see Line 73.

8. - L. 69: "The limited knowledge of including or not complex vadose zone processes: : :" Please clarify this sentence.

Response: Here the complex vadose zone processes is referring to the "explicit consideration of ice effect, water and heat coupling". We want to say that there has not been too much effort investigating the role of the increasing complexity of soil physical processes in cold region ecosystems. we rephrased it as "The inclusion or exclusion of different soil physical processes, i.e., explicit considering ice effect and tightly coupled water and heat transfer, in such environment frames the scope here." See Line 80.

9. Methods: The model descriptions in the methods are somewhat unstructured and in part difficult to follow. I see the value of presenting the equations, but I would suggest to introduce the three model setups in the beginning of the methods section, and to describe the processes and equations per setup.

For the numerical experiments (section 2.6), please specify which driving variables were used and at which temporal resolution, and how the initial state of the model was determined – without understanding the driving variables of the model, it is hard to evaluate the performance.

Response: The method part regarding the model descriptions has been modified accordingly. We first present the soil physical processes used in T&C, T&C-FT, and STEMMUS model in Section 3.1-3.4. Then the coupling T&C and STEMMUS procedure is introduced in Section 3.4, followed by the design of numerical experiments in Section 3.5.

The description of driving variables was added in Section 3.5 as "Hourly meteorological forcing (including downwelling solar radiation, precipitation, air temperature, relative humidity, wind speed, atmospheric pressure) was utilized to drive the models. For the adaptive time step of STEMMUS simulation, linear interpolation between two adjacent hourly meteorological measurements was used to generate the required second values."

10. - L. 101: Please specify whether you use remote sensing data for one pixel only, or whether you use it for a spatial analysis, and what it hence is "representative" (L. 102) for.

Response: As the lack of in situ measurements of time series of vegetation dynamics, here we intended to use remote sensing data (MCD15A3H and MOD17A2H) as the auxiliary data for the vegetation dynamics of the in situ site (corresponding to the central experimental site (33°54′59″N, 102°09′32″, elevation: 3430m)). One pixel data corresponding to the study location was employed here in terms of the spatial scale. We rephrased the "representative" with "We downloaded MCD15A3H (Myneni et al., 2015) and MOD17A2H (Running et al., 2015) products for this site as the auxiliary vegetation dynamics data". See Line 126.

11. - Fig. 1b: It is hard to interpret the freezing front data, in particular for winter 2017-18 because of the missing data. Is it possible to mark the times and depths of missing data? Also, smaller symbols in the figure would probably allow to differentiate the dynamics at the surface better.

Response: Figure 2b (original Figure 1b) was replotted accordingly. Here we generated the dynamics of freezing/thawing front by interpolating the measured soil temperature data at soil depths of 2.5, 5, 10, 20, 60, and 100cm, neglecting 40cm (at which depth the data is missing for 2017-18 winter). The missing data periods of soil moisture/temperature measurements were described in the text.

Changes in the manuscript: "Note that there are data gaps (25th Mar – 8th June, 2016; 29th Mar – 27th July, 2017, extended to 12th Aug, 2018 for 40 cm) due to the malfunction of instruments and the difficulty to maintain the network under harsh environment. "see Line 123.

12. - For the subscripts used in the equations, please separate the i used for layering (Eq. 2) from the i used for ice (Eq. 3, L. 196, Eq. 5).

Response: We made modifications as: 'i 'is specifically used for layering and 'ice' is used for soil ice (changes can be found as Eq. 4, Eq. 6, L. 233, Eq. 7, Eq. 8).

13. - Eq. 4: Please check this equation: the left-hand side is mass-based, and the righthand side volume-based. I assume that soil density should be added to the equation.

Response: Many thanks for pointing it out. Eq. 4 (now Eq. 3): We added the soil density term (ρ_{soil}) in Eq. 3, making the left-hand side consistent with the right-hand side both as volume-based terms. In addition, such modifications are made in Eq. 6 & 8.

14. - L. 235: Convergence of which variables, and which criterion is used to determine if convergence has been achieved?

Response: The iteration solution is used in STEMMUS to solve the soil moisture and temperature states. The convergency criteria are both set as 0.001 for soil matric potential and soil temperature.

Furthermore, the maximum desirable change of soil moisture and soil temperature within one step was set as 0.02 cm³ cm⁻³ and 2 °C, respectively, to prevent too large change in state variables that may cause numerical instabilities. If the changes between two adjacent soil moisture/temperature states are less than the maximum desirable change, then STEMMUS continues without changing time step. Otherwise, STEMMUS will adjust the time step and repeat the current time step. During the freezing/thawing transition periods, we added the additional constraint on the time step to keep the smooth change of soil energy content. By decreasing the time step, the soil temperatures from two adjacent iterations were ensured either greater (smaller) than or equal to the freezing temperature (i.e., heating, cooling or zero-curtain effect).

Changes in the manuscript: "After convergence is achieved in the soil module (i.e., convergence criteria is set as 0.001 for both soil matric potential [in cm] and soil temperature [in K])" see Line 257.

15. The energy fluxes displayed in Fig. 3 and 4 are too large, probably by a constant factor (the seasonal dynamics look fine), resulting in fluxes that exceed theoretical limits set by incoming radiation – please check the averaging method. Numbers in Fig. 9 seem more realistic.

Response: Thanks a lot for pointing it out. In the original Fig. 3 and 4, we used wrong units summing values of hourly surface energy fluxes (ranging from -500 to 1000 W/m² for net radiation) into daily

values. For the updated Fig. 4 and 5, we corrected the mistake and we properly averaged the surface energy fluxes at the daily time scale then presented the 5-day moving average values of surface energy fluxes (ranging from -20 to 200 W/m² for net radiation).

For Fig. 10 (original Figure 9), the hourly values of surface energy fluxes, plotted as the scattered figures between the observed and model simulated values, were used to indicate the energy balance closure problem.

We made some modifications in captions of Figures 4, 5 and Figure 10 to clearly indicate whether hourly or daily average values are used.

16. In general, the analysis focuses on the entire period of simulation. This is fine for a general overview, but differences between the three model versions tend to be small for most of the period. I would recommend focusing on specific times of the year where the three model versions deviate, and discuss the abilities of the three models for these periods specifically. Also, the authors could consider displaying differences from observations rather than absolute amounts, to make differences between model versions more visible. At the moment, the main conclusion that one draws as reader is that the choice of model version does not matter too much, whereas the differences between the model versions may well provide important insights e.g. in representing fluxes during freezing times.

Response: Thanks for the suggestion. We added additional figures in the supplement materials to highlight differences in specific periods (see supplement Figures S1-3). We zoomed in a new figure (Fig. S1) in the frozen period and we showed the relative differences between observations and model simulations. We add an appropriate reference in the manuscript and supplement accordingly.

17. - Can the authors comment on the differences in the models' abilities to capture LE and H? The model is doing a very good job in capturing LE, but variations in H are poorly captured. Regarding the "overall performance:::in terms of turbulent flux simulation", I think this difference between LE and H should be noted. Also, the models simulate consistently a large difference in H between the summer from 2017 and those from 2016 and 2018, whereas observations indicate less variations between summers. What is the reason for the simulated differences between 2016 and 2018 on the one hand and 2017 on the other?

Response: It is difficult to attribute such a difference mostly to the model inaccuracy or mostly to the data inaccuracy. On one hand, the energy balance closure problem rises as the potential source of error and reason of discrepancy. The Eddy covariance observed LE and mostly H fluxes are underestimated when constrained by the surface energy closure during the summer periods (see Table 2). On the other hand, in T&C model, surface temperature is simplified and 'one single prognostic surface temperature' is computed, i.e. soil surface and vegetation surface temperature have the same value. The difference between the soil surface, vegetation surface and the assumed surface temperature can be a potential cause for such discrepancies in *H*.

In addition, soil moisture and temperature simulation fit changes corresponding to that of surface energy fluxes simulations (i.e., slightly better in 2017 than that in 2016 and 2018, see Fig. 6). The uncertainties in the precipitation measurements thus can be an additional potential reason for the simulated differences between 2016 & 2018 and 2017. All these aspects are well explained in Sect. 4.1.

18. - L. 304 and Fig. 7ab: What causes the pronounced difference in simulated ice content between the two model versions, and is the band of high ice content in unCPLD-FT in the first winter season a model artefact or a real phenomenon? For comparing, it would be preferable to have the same colour scale for plots 7a and 7b.

Response: Soil ice content measurements are not easy to achieve in the field. It is hard to accurately assess the model performance regarding the soil ice content simulations. We simply rely on the freezing/thawing front propagation to validate the general spatiotemporal shape of soil ice content dynamics.

For the band of high ice content in unCPLD-FT in the first winter season, this is generated by cryosuction of liquid water in the upper soil layers. The freezing-induced water potential decrease moves the available liquid water towards the freezing front. The high accumulation of ice content indicates that unCPLD-FT model simulated a relatively strong cryosuction effect, probably mitigated in the fully coupled model by effects of water vapor transfer and thermal gradients, as well as different solutions in the parameterization of soil-freezing curves.

We now used the same colour scale for Figure 8a &b (original Figure 7).

Changes in the manuscript: "It is to note that compared to unCPLD-FT model, CPLD model presented a relatively lower presence of soil ice content, while its temporal dynamics was closer to the observed freezing/thawing front propagation. The difference between the two simulations can be attributed to the constraints imposed by the interdependence of liquid, ice, and vapor in the soil pores that is considered only in CPLD model." see Line 359.

19. - L. 326: What causes the difference in onset between unCPLD and CPLD on the one hand and unCPLD-FT on the other? How do the soil physics processes impact GPP?

Response: The onset of vegetation depends on the soil temperature in the root zone averaged over the previous 30 days. For the first winter season, unCPLD-FT model simulated a prolonged freezing period than unCPLD and CPLD model. Thus, there is a delay in the vegetation onset date. For the second winter season, all three models produce similar vegetation onset dates. For the third winter season, more spread was detected among the three model simulations. unCPLD produced the earliest onset date while unCPLD-FT produced the latest onset date, with CPLD fell in between.

The difference in soil physics processes alters the soil liquid water/temperature profile simulations and especially the strong cryosuction effect in the unCPLD-FT generates larger ice accumulation and a delay in

the melting that leads to lower average temperatures. These processes affect the leaf onset date, i.e., the phenology of the grassland. Additionally, the changes in soil liquid water content can result in variations of water stress for the plants, thus they affect the photosynthetic assimilation rate and GPP. Differences in soil temperature profiles can also affect root respiration in generating additional small differences in GPP.

Changes in the manuscript: "The difference in the soil liquid water/temperature profile simulations between the CPLD and unCPLD models (as shown in Figures 6 & 7) resulted in differences in simulated vegetation dynamics, especially concerning the leaf onset date, which is affected by integrated winter soil temperatures. The unCPLD-FT model has a delay in the vegetation onset date when compared to other simulations, due to the significant cryosuction that prolongs freezing conditions and keep lower soil temperatures. This makes the unCPLD simulation having slightly shorter vegetation active season compared to the CPLD model simulations. The lower GPP in the unCPLD simulations is instead related to a slightly enhanced water-stress induced by the different soil-moisture dynamics during the winter and summer season with a lower root zone moisture produced by the unCPLD model (Figure 6), which affects the plant photosynthesis and growth. Differences in soil temperature profiles can also affect root respiration in generating additional small differences in GPP." see Line 392.

20. The discussion is generally fine and provides insights in how soil physics processes are expected to affect other parts of the ecohydrological system. It would be nice to see whether conclusions from the authors corroborate existing literature, and where they agree. The conclusion provides a balanced assessment of the advantages and disadvantages of enhanced model complexity for representing the dynamics.

Response: We thank the reviewer for this perspective. Additional references were added in the discussion part to expand it. For example, the 10yr CO2 fluxes observation in an alpine shrubland on the Qinghai-Tibetan Plateau by (Li et al. 2016) aligns well with this study as it indicated that the non-growing season soil temperature can exert important effects on the carbon flux dynamics, as it can enhance the vegetation activities and prolong the growing season.

21. - L. 361: Specify which slope is discussed here (it is clear from the figure, but hard to understand from the text).

Response:. We added the description text here to specify the meaning of slope as "The sum of measured LE and H was significantly less than Rn, with the slope of *LE+H* versus Rn equal to 0.59 (Fig. 10a)." see Line 409.

22. The language would benefit from editing by a native speaker. Also, references should be checked carefully; references seem to be missing from the reference list (Fisher et al. 2014) or need to be specified (Yu et al. 2016a and 2016b in the reference list, but the text refers to Yu et al. 2016).

Response: We carefully checked the references and made it consistent between the text and reference list. References (Fisher et al. 2014) were added to the reference list. As the changes in the introduction part, Yu et al. 2016a were no longer there. Accordingly, the newly added references were inserted both in the context and the reference list. The English grammar and fluency have been re-checked carefully throughout the entire manuscript.

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Referee #2

General Comment: "How vadose zone mass and energy transfer physics affects the ecohydrological dynamics of a Tibetan meadow?" by Yu et al. addresses the importance of including freezing and thawing processes and coupling water and energy balance equations of vadose zone models to simulate ecohydrological dynamics. The authors use data from a high-elevation meadow of the Tibetan plateau to evaluate the outcomes of their different simulations. From their results, the authors claim that adding model complexity improves the model estimates of soil temperature and moisture but may not be necessary to model vegetation dynamics in these regions.

The manuscript is generally well written and understandable. While the presentation and interpretation of the results makes sense, it sometimes lacks clarifications and could benefit from a deeper analysis. I think the model, even fully coupled, does a poor job at reproducing ice content and thermal conditions of deeper layers. As pointed by the authors, some data collected to evaluate the different simulations seem wrong, while others are simply missing, which means it can be barely used to validate any of the simulations. However, the conclusions of this manuscript remain valid and of considerable interest and is valuable to anyone wondering about the importance of including dynamic freezing and thawing processes in their models. Overall, this manuscript has the potential to be an interesting and useful contribution to The Cryosphere, but some critical issues, mostly in the methodology section, need to be addressed before considering publication.

I also think this manuscript does not reach its full potential. It could use various level of complexity in their approach to include freezing and thawing processes. For example, the CPLD simulation could be divided into different simulations: one that only considers latent heat, one that only considers the effect of ice content on the hydraulic conductivity, etc. This would show modelers which component of the freezing/thawing processes is important to consider, and which one is potentially not. However, I acknowledge that this suggestion would involve substantial additional work, so I understand if the authors would rather not make this change. Here are my detailed comments.

Response: Many thanks for your constructive comments. We made modifications of the methodology section, in which the clear writing flow was followed. The governing equations and main constitutive equations for different models were clearly presented. The differences among three models regarding soil physical processes were illustrated in Table 1 and Sect. 3.5. The constitutive equations of unfrozen water content, temperature dependence of liquid flow, the ice effect on hydraulic conductivity, and water vapor density was presented in supplement material (Section S1). We added the geographical location of the Maqu soil moisture and temperature monitoring network and the central experimental site (Figure 1, thus the original figure number was changed). In addition, the description of data gaps was briefly presented.

We appreciate your suggested simulations on investigating which component of the freezing/thawing processes is important. This question indeed can be investigated in our future work. We would rather not making this change right now though, and want to present the current results step by step to avoid overwhelming information in one manuscript.

1. Introduction: Well written and introduce well the topic and the problematic. However, I think the authors could add a few lines about the efforts done so far to model freezing and thawing processes in coupled water & energy models for cold regions. There are numerous subsurface and surface models already doing that. They do not all necessarily simulate ecological dynamics, but some studies have provided useful information about the impact of neglecting freezing dynamics.

Response: Thanks a lot for your suggestions. We added in the first part of Introduction some studies that evaluate the modeling of freezing and thawing processes coupled water and energy and pointed out that the novelty here is that also ecohydrological dynamics are jointly evaluated.

Changes in the manuscript: "Concurrently, researchers developed dedicated models, e.g, SHAW (Flerchinger and Saxton, 1989), HYDRUS (Hansson et al., 2004), MarsFlo (Painter, 2011), and STEMMUS-FT (Yu et al., 2018), considering the soil water and heat coupling physics for frozen soils. Promising simulation results have been reported for the soil hydrothermal regimes. While these efforts mainly focus on understanding the surface and subsurface soil water and heat transfer process (Yu et al., 2018) and stress the role of physical representation of freezing/thawing process (Boone et al., 2000; Wang et al., 2017b; Zheng et al., 2017), they seldom take into account the interaction with vegetation and carbon dynamics."

2. L56: Unclear what is meant by "changes of frozen ground". Maybe the authors meant something like "variations in seasonally frozen ground thickness"?

Response: Yes, here it is meant to be "variations in seasonally frozen ground thickness". Corrected in the manuscript. See Line 69.

3. L58: What are those divergences? Please provide a few examples.

Response: We added some examples here.

Changes in the manuscript: "However, there are divergences with regard to the expected ecosystem changes across the Tibetan Plateau (Cheng and Wu, 2007;Qin et al., 2016;Wang et al., 2018;Zhao et al., 2010). In response to climate warming, the degradation of frozen ground can positively affect the vegetation growth in Tibetan Plateau mountainous region (Qin et al., 2016), but it can also lead to degradation of grasslands (Cheng and Wu, 2007), depending on soil hydrothermal regimes and climate conditions (Qin et al., 2016;Wang et al., 2016). "see Line 71.

4. L70: I am not sure "complexity" is the best word here. According to the authors, they are testing their models with or without freezing dynamics, and with or without water and energy coupling. As I understand it, there are no different "complexities" in the way frozen soil is represented or in the way the coupling is achieved.

Response: Here we intended to say that the vadose zone water and heat transfer physics is represented in an increasingly complex way (from the T&C without the freezing dynamics, with freezing dynamics but uncoupled water and heat transfer, to the coupling of T&C with STEMMUS to account for fully coupled processes).

For unCPLD model (T&C), soil water and heat are independently simulated, ice effect is not considered.

For the unCPLD-FT model (T&C-FT), the ice effect on hydraulic conductivity is considered via an impedance factor; thermal conductivity and capacity are affected by the ice content; latent heat change during the freezing/thawing period is taken into account but heat does not exchange with liquid water. During the non-frozen period, soil water and heat are still independently transferred.

For the CPLD model (T&C-STEMMUS), the ice effect on the hydrothermal properties is considered; latent heat change from the freezing/thawing process is also taken into account. Vapor flow, which links the soil water and heat flow, is simulated. The thermal effect on water flow is explicitly considered. Thus, soil water and heat transfer processes are tightly coupled not only during the frozen period but also during the non-frozen period for the CPLD model.

We better explained these aspects in Sect. 3.5.

Changes in the manuscript: "To investigate the role of increasing complexity of vadose zone physics in ecosystem functioning, three numerical experiments were designed on the basis of the aforementioned modeling framework (Table 1). First experiment, the T&C original model was run as stand-alone, termed as unCPLD simulation. For the unCPLD model, soil water and heat transfer is independent with no explicit consideration of soil ice effect. The second experiment, the updated T&C model with explicit consideration of freezing/thawing process was run as it can estimate the dynamics of soil ice content and the related effect on water and heat transfer (e.g., blocking effect on water flow, heat release/gain due to phase change) but otherwise being exactly equal to T&C original model. This second simulation is named the unCPLD-FT simulation, where the term unCPLD generally refers to the fact that T&C model and STEMMUS model are not yet coupled. The third experiment, STEMMUS model was coupled with T&C model to enable not only frozen soil physics but also additional processes and most importantly the tight coupling of water and heat effects. This simulation is named CPLD simulation. In this third scenario, vapor flow, which links the soil water and heat flow, is explicitly considered. In addition to the ice blocking effect as presented in unCPLD-FT, the thermal effect on water flow is also expressed with the temperature dependence of

hydraulic conductivity and matric potential. Furthermore, not only the latent heat due to phase change, but also the convective heat due to liquid/vapor flow is simulated. "

5. Section 2.1: It is unclear until the reader reaches the results section if the experimental site is underlain by permafrost or not. Please add somewhere in this section that the site only has seasonally frozen ground.

Response: We added this information in the text in Sect. 2.1 as "Seasonally frozen ground is characteristic of this site, with the maximum freezing depth approaching around 0.8 m under current climate conditions." See Line 121.

6. L 93: It is written here that the SMST profiles are measuring temperature and soil moisture at a depth of 80 cm. However, figures from the results section are never showing data at 80 cm, only at 60 cm (which is not listed in line 93). Please fix or clarify.

Response: For Maqu soil moisture and soil temperature (SMST) monitoring network, the SMST profiles are generally measured at depths of 5 cm, 10 cm, 20 cm, 40 cm, and 80 cm. In addition, we have installed some additional 5 TM ECH2O probes to enrich the SMST profile information at specific points. Here, the additional SMST profiles, installed at 2.5 cm, 5 cm, 10 cm, 20 cm, 40 cm, 60 cm, and 100cm, were employed for validating the model simulations. We clarified this point in Sect. 2.1.

Changes in the manuscript: "A few dedicated SMST profiles, with sensors installed at depths of 2.5 cm, 5 cm, 10 cm, 20 cm, 40 cm, 60 cm, and 100 cm, were used for validating the model simulations." See Line 122.

7. Figure 1b: If the figure is indeed showing both freezing and thawing fronts, I would recommend using different colors. It is unclear which zone is thawed and which one is frozen (mostly in 2017-2018). I also think the y-axis should not reach 100 cm. Based on the text, there is no sensor deeper than 80 cm. If I understood correctly, the graph is plotting information the authors do not have. Please fix or clarify in the text. Furthermore, is the data here interpolated from the 5 sensors described in line 93?

Response: Different colors are now presented in Figure 2b, with the freezing fronts color blue and thawing fronts color red. In the updated Figure 2b, soil temperature measurements at depths of 2.5 cm, 5 cm, 10 cm, 20 cm, 60 cm, and 100 cm were used to generate the freezing/thawing front propagation dynamics. Soil temperature measurements at 40cm are not used as its large data gaps during 2017-2018 wintertime (see Table R.1).

Table R.1. The main data gaps for soil moisture/soil temperature (SMST) measurements

SMST	Data gaps		

```
2.5 cm 3/25/2016 - 6/8/2016, 3/29/2017 - 7/27/2017

5 cm 3/25/2016 - 6/8/2016, 3/29/2017 - 7/27/2017

10 cm 3/25/2016 - 6/8/2016, 3/29/2017 - 7/27/2017

20 cm 3/25/2016 - 6/8/2016, 3/29/2017 - 7/27/2017

40 cm 3/25/2016 - 6/8/2016, 3/29/2017 - 8/12/2018

60 cm 3/25/2016 - 6/8/2016, 3/29/2017 - 7/27/2017

100 cm 3/25/2016 - 6/8/2016, 3/29/2017 - 7/27/2017
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Changes in the manuscript: "A few dedicated SMST profiles, with sensors installed at depths of 2.5 cm, 5 cm, 10 cm, 20 cm, 40 cm, 60 cm, and 100 cm, were used for validating the model simulations. Note that there are data gaps (25th Mar – 8th June, 2016; 29th Mar – 27th July, 2017, extended to 12th Aug, 2018 for 40 cm) due to the malfunction of instruments and the difficulty to maintain the network under harsh environment."

8. L 124: Please provide more information about the missing data. When and where? This should also be shown in Figure 1b. For example, the authors can use a greyed area to show where data are missing. This is crucial considering the authors are using this data or comparison purposes in Figure 6.

Response: The main data gaps for SMST measurements are summarized as Table R.1. For Figure 1b, the propagation of freezing/thawing front was obtained by interpolated the SMST profile measurements (2.5 cm, 5 cm, 10 cm, 20 cm, 60 cm, and 100 cm). Here, soil temperature measurements at a depth of 40 cm were omitted as its long data gaps during the second winter period (2017-2018).

Changes in the manuscript: "Note that there are data gaps (25th Mar – 8th June, 2016; 29th Mar – 27th July, 2017, extended to 12th Aug, 2018 for 40 cm) due to the malfunction of instruments and the difficulty to maintain the network under harsh environment."

9. Equation 1: Check units. Are the units of S really s-1 or rather kg m-3 s-1?

Response: The unit of S, the sink term, is kg m⁻³ s⁻¹ with the consideration of water density. We corrected the unit of S as 'kg m⁻³ s⁻¹'.

10. Equation 2: Undefined variables: dz, rH, rL, nc

Response: Equation 2: Note that to avoid confusion, the terms not used in this simulation case was deleted from Eq. 2. We added the relevant description.

Changes in the manuscript:

$$d_{z,i}\frac{d\theta_i}{dt} = q_{i-1} - q_i - T_v r_{v,i} - E_s - E_{bare}$$
(2)

where $d_{z,i}$ (m) is the thickness of layer i; q_i (m s⁻¹) is the vertical outflow from a layer i; T_v (m s⁻¹) is the transpiration fluxes from the vegetation; $r_{v,i}$ is the fraction of root biomass contained in soil layer i; E_{bare} (m s⁻¹), evaporation from the bare soil; E_s (m s⁻¹), evaporation from soil under the canopy.

11. Equation 4: Csoil is presented as the specific heat capacity of the bulk soil, but I think it is the volumetric heat capacity. The units do not match otherwise. The same issue arises in equations 6, 7 and 8. Equation 8 is from Hansson et al. (2004), where Csoil is defined as the volumetric heat capacity.

Response: Many thanks for pointing out this. Equation 4: There was an inconsistency between the left and right side of Equations 4, 6, 7, and 8 (now Eqs. 3, 4, 5, 6). We multiplied Csoil with the soil density ρ_{soil} to make it consistent. Capp was clarified as the apparent volumetric heat capacity here as Equation 8 (now Eq. 5).

12. Equation 8: Please define which phase is represented by $d\theta$. It should be liquid water.

Response: Thanks a lot for your comment. We added some text as "differential (specific) water capacity $d\theta/d\psi$ at a given liquid water content θ ". (now Equation 6, Line 198)

13. Section 2.4.4: The authors describe in detail the equations of the two models but do not explain the critical components of the added freezing/thawing processes, except for latent heat. They do provide references but, considering that this is supposedly an important aspect of this manuscript, they should at least describe in more details the different equations used. For example, the calculation of the hydraulic conductivity for a frozen medium is quite important. The authors refer here to Hansson et al. (2004), which uses an impedance factor. This method is widely used, but the impedance factor is an arbitrary number that is likely to change based on the type of soil. The authors never write which impedance factor is used. I am also concerned that the authors are using the method from Dall'Amico et al. (2011) for the soil freezing characteristic curve and the method from Hansson et al. (2004) for the apparent heat capacity. These two papers both use a form of the Clausius-Clapeyron equation with the van Genuchten model, but with different approaches. I could be wrong but, depending on how they have been used, these two methods may not be compatible with each other. More information is required here to make sure the freezing model used by the authors is valid.

Response: We added the description of the freezing/thawing process, i.e., how unfrozen water content, hydraulic conductivity is calculated, the assignment of impedance factor, temperature dependency of hydraulic conductivity/matric potential, vapor density parameterization. As this information does not represent the main physical equation but rather parameterizations, we did not list them in the main text but in the supplemental materials (Supplement S1).

The apparent heat capacity is calculated as $C_{app} = \rho_{soil}C_{soil} - \rho_{ice}L_f \frac{\partial\theta_{ice}}{\partial T}$ to express both the heat conduction and latent heat (phase change) terms. On the basis of the assumption of zero ice gauge pressure and osmotic pressure, Clausius-Clapeyron equation is utilized to convert $-\rho_{ice}L_f \frac{\partial\theta_{ice}}{\partial T}$ into $\rho_{ice} \frac{L_f^2}{gT} \frac{d\theta}{d\psi}$. This is a general procedure to derive the apparent heat capacity and it is independent of which form of the soil-freezing characteristic function is used. The assumption and the Clausius-Clapeyron equation used in Dall'Amico (2011) is the same as Hansson et al. (2004) (i.e., $\frac{dP}{dT} = \frac{L_f}{V_W T}$), there is no difference between these two papers in calculating the apparent heat capacity.

The beauty of the equation (19) – (21) in Dall'Amico et al., (2011) - the equations used to estimate the additional freezing pressure due to the unfrozen water pressure - is that they are fully energy conservative (contrary to other formulations) and are also independent of the specific hydraulic parameterization of the soil (even though later on van Genuchten method is used in Dall'Amico et al. 2011). As a matter of fact, in T&C-FT, three different soil hydraulic parameterizations can be used: (i) van Genuchten, (ii) Saxton-Rawls and (iii) Clapp and Hornberger. For all of these the liquid water pressure is derived with equation (21), but then the actual liquid and frozen water content depend on the specific soil hydraulic parameterization chosen. Before implementing the Dall'Amico et al., (2011) formulation, we had a lot of problems related to energy conservation in the freezing/melting phases, problems that were not apparent for a week-ten days of simulations but developed over time, so we checked carefully that energy is indeed properly conserved in the long-term in T&C-FT.

Changes in the manuscript: "The soil freezing characteristic curve providing the liquid water potential in a frozen soil is computed following the energy conservative solution proposed by Dall'Amico et al. (2011) and it can be combined with various soil hydraulic parameterizations including van Genuchten and Saxton and Rawls to compute the maximum liquid water content at a given temperature and consequently ice and liquid content profiles at any time step (Fuchs et al., 1978; Yu et al., 2018)." See Line 201.

14. Section 2.6: I think this section lacks some important clarifications. First, I think the differences between the models are more complicated than coupled/uncoupled. The vadose zone equations of T&C model are not coupled, because the water and heat equations are independent from each other. On the other end, the heat equation of STEMMUS needs to be coupled to the mass transfer equation because of the consideration of different processes or constituents such as heat advection. However, when adding the freezing/thawing processes, the heat and water equations of T&C becomes somehow coupled (at least one-way) due to the temperature dependency of the hydraulic conductivity. It is unclear if the authors used the names unCPLD, unCPLD-FT and CPLD for their models to characterize the way the heat and water equations are solved or to characterize how the two components (T&C and STEMMUS) are used. If it is the former, I suggest that they authors rename their simulations as T&C, T&C-FT and T&C-STEMMUS. In any case, the coupling characteristics of the different simulations should be further

explained. Secondly, it is unclear which processes/parameters are considered in each simulation. For example, the authors state in the discussion that "unCPLD-FT simulation accounting for soil-freezing in a simplified way in comparison to STEMMUS (e.g., the CPLD simulation)" (line 418-419). However, to my knowledge, the difference in the way STEMMUS accounts for soil-freezing processes is never explained. A paragraph describing the different processes that each simulation is accounting for is necessary in this section. This can also take the form of a table.

Response: Thanks a lot for the comment. Yes, the "coupling" in the label was referring to the coupling among models rather than in the processes. In order to present the difference among the model versions and clarify the words 'unCPLD, CPLD', we added Table 1 and relevant descriptions in the Sect. 3.5 to explain the difference and the processes considered in each simulation case.

15. Figure 3: The grey line is hard to distinguish. I suggest making it slightly darker or thicker.

Response: We made the grey line darker and thicker in Figure 4.

16. Figures 5 and 6: It looks like deeper soil moisture and temperature is not well reproduced by any of the models, even though it is not discussed in the text. This has the consequence of poorly representing ice content (Figure 7), mostly in 2017-2018. It is understandable considering the model has not been calibrated and the goal of this manuscript, which focuses more on the growing season, is not necessarily to validate the models. However, I think this poor fit with field measurement should be discussed in the text. There are many reasons that could explain this, such as the presence of heterogeneity in the soil or of freezing-point depression due to increased salinity.

Response: In Sect. 4.2, We now discussed the reasons for the discrepancies between the model simulated and observed soil moisture and temperature at deeper soil layers.

Changes in the manuscript: "It should be noted that for the deeper soil layers (e.g., 60cm in Figure 7), all models tended to simulate the early start of freezing soil temperatures and considerably underestimated the soil temperature during the frozen period. This can be due to the uncertainties in soil organic layer parameters, the not fully captured snow cover effect (Gouttevin et al., 2012), a potentially pronounced heterogeneity in soil hydrothermal properties, or the potential role of solutes on the freezing-point depression (the presence of solute lowers the freezing soil temperature) (Painter and Karra, 2014). These mismatches in deep soil temperature degraded the model performance in simulating the dynamics of liquid water (Figure 6) and ice content (Figure 8) during the frozen period. "

17. L 303: I think they authors meant "unCPLD-FT" instead of "unCPLD".

Response: We initially used "unCPLD" model simulations to refer to both the "unCPLD" and "unCPLD-FT" model simulations, as Fig. 8 also presents the water flow simulations of unCPLD model. To avoid confusion, we rephrased this sentence as "The time-series of soil ice content and water flux from unCPLD,

unCPLD-FT and CPLD model simulations for soil layers below 2 cm are presented in Figure 8." See Line 349.

18. L 307-309: I do not agree that the CPLD model shows a good match with field measurements of ice content, at least not as currently showed in winter 2017-2018.

Response: Yes. Both the unCPLD and CPLD model cannot well reproduce the soil ice content based on current simulations. Here, we would like to stress the difference between unCPLD-FT and CPLD model. CPLD model presents a shallower freezing ice depth compared to unCPLD-FT model. We attributed this to the physical difference between unCPLD-FT and CPLD model, i.e., the constraints by the interdependence of liquid, ice, vapor, air components in the soil pores are considered by CPLD model.

Changes in the manuscript: "It is to note that compared to unCPLD-FT model, CPLD model presented a relatively lower presence of soil ice content, while its temporal dynamics was closer to the observed freezing/thawing front propagation. The difference between the two simulations can be attributed to the constraints imposed by the interdependence of liquid, ice and vapor in the soil pores that is considered only in CPLD model." see Line 359.

19. Figure 8: Please define acronyms in the caption (e.g., "(a) Gross Primary Production" instead of "(a) GPP")

Response: We describe acronyms in the caption of Figure 9.

Changes in the manuscript: "Figure 9. Comparison of observations from Eddy Covariance (OBS) or MODIS remote sensing and simulated (a) Gross Primary Production (GPP), (b) Leaf Area Index (LAI), (c) Net Ecosystem Exchange (NEE), and (d) Ecosystem respiration (Reco) using unCPLD, unCPLD-FT, and CPLD model. MODIS refers to the data from MODIS-GPP and MODIS-LAI products."

20. Figure 9: The authors use R2 here and R in Figure 8. I suggest them to choose one and be consistent.

Response: Yes, sorry for the confusion. We use the determination coefficient R² and keep it consistent in Figure 5 and Figure 10.

21. Figure 10: Please define acronyms in the figure caption.

Response: We added the descriptions of the acronyms as "Tv, transpiration; Es, surface evaporation; E_{IN} and E_{SN} , evaporation from intercepted canopy water and snow cover; ΔVs , changes in soil water storage; L_K , deep leakage water.".

22. L 381-382: Confusing sentence. Should we compare to unCPLD or unCPLD-FT?

Response: Here we compare unCPLD model simulations with unCPLD-FT model simulation to highlight the role of ice content and latent heat associated with phase change only. This has been clarified as "Less amount of water was consumed by ET from unCPLD-FT simulations than that from unCPLD." See Line 429.

23. L 383-384: What could explain cooler late winter temperatures in unCPLD-FT? Latent heat slowing down the thawing? Lower bulk heat capacity of frozen soil? Please provide hypotheses.

Response: As for unCPLD-FT model, the effect of ice content and latent heat due to phase change were taken into account, while these two effects were absent by unCPLD model. During the late winter (mainly thawing periods), the thawing process was retarded by the heat absorption due to phase change. Secondly, the ice induced soil heat capacity also damped the magnitude of temperature variations, make the thawing process of soil temperature more difficult and slower. Generally, as discussed earlier there is a quite evident cryoscution in the unCPLD-FT simulation that generates a considerable amount of ice content in the soil that takes time to be melt and reduce the average temperature. Thus there are cooler late winter temperatures in the unCPLD-FT model than in the unCPLD simulations.

Changes in the manuscript: "The cooler late winter temperatures from unCPLD-FT simulations can be attributed to the retardation of the thawing process due to the phase change-induced heat absorption and the soil ice-induced modification of bulk heat capacity during the freezing-thawing transition period, which damped the magnitude of temperature variations and delayed the thawing process." See Line 432.

24. L 396-400: This analysis could be improved. The coupling is not the only difference between CPLD and unCPLD-FT. STEMMUS is simulating some subsurface processes that T&C does not (e.g., heat advection, air flow, vapor flow). I recommend providing a more detailed analysis then simply justifying the differences by the coupling. Also, how is ice content and hydraulic conductivity being simulated differently in CPLD than in unCPLD-FT?

Response:. We agree with your points that the coupling is not the only difference between CPLD and unCPLD-FT model. These contexts (L396-400) were used to explain why the water storage amount in the vadose zone is increased while the bottom leakage decreased for CPLD model (Figure 11). It lies in the difference of the considered subsurface processes between CPLD and unCPLD models (Sect. 3.5, Table 1). We further described the hydraulic conductivity (and its temperature dependency), vapor density in supplement S1.

Hydraulic conductivity in CPLD (T&C-STEMMUS) model is dependent on temperature in two ways. 1. The impedance effect of soil ice content on the hydraulic conductivity, which is dependent on soil temperature, (i.e., reducing the saturated hydraulic conductivity via an empirical impedance factor). 2. The water viscosity effect on hydraulic conductivity. As the temperature decreases, water movement slows down.

Changes in the manuscript: "We attribute this to the way ice content is simulated in the CPLD simulation, and also to the temperature dependence of soil hydraulic conductivity (see Table 1 and Supplement S1). Specifically, the high accumulation of ice content in the unCPLD-FT simulations indicates a relatively stronger cryosuction effect than in CPLD simulations. This cryosuction effect is mitigated in the fully coupled model because of water vapor transfer and thermal gradients, even though different solutions in the parameterization of bulk soil thermal conductivity and volumetric soil heat capacity could also be responsible for the difference. Overall, taking into account the fully coupled water and heat physics modify the temporal dynamics of ice formation and thawing in the soil and activates temperature effects on water flow (i.e., low soil temperature will slow down water movement)." See Line 447.

25. L 407-410: There are two requirements to experience heat advection: water flow and difference in temperature. While the former is shown in Figure 7, there is no evidence shown for the latter. It would be interesting if the authors could provide some evidence (can be with numbers or words) that heat advection (or convective heat) is mostly relevant during the frozen period.

Response: Here, we highlight the difference between unCPLD and CPLD models on heat advection effects. As shown in Figure 8c and d/e, the difference in water flow can be several orders of magnitude. We added some references here to corroborate this point.

Changes in the manuscript: "The liquid water flux-induced convective heat flux is mostly relevant during the frozen period (Boike et al., 2008; Kane et al., 2001; Yu et al., 2020). As it has been observed, a certain amount of liquid water/vapor flux moving toward the freezing front and this effect is different between unCPLD-FT and CPLD while absent in unCPLD (Figure 8). For the unfrozen period, instead, the total mass fluxes were comparable between the two unCPLD and CPLD simulations. For the temperature gradient, there is not much difference between unCPLD and CPLD simulations during both the growing season and frozen period." See Line 461.

26. L 413: I think Figure 8 should be referred here instead of Figure 9.

Response: Yes sorry. The number of figure was changed as we added the geographical figure. We corrected it in the manuscript (Line 470). Thanks a lot.

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How On the Role of vadose Vadose zone Zone mass and energy transfer pPhysics affectins the ecohydrological Ecohydrological dynamics—Response of a Tibetan meadow Meadow? to Freeze-Thaw Cycles

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Abstract. The vadose zone is a sensitive region zone to environmental changes and exerts a crucial control in ecosystem functioning, and even more so in cold regions with seasonally frozen ground. While the way in representing the underlying physical process of vadose zone differs among models, the effect of such differences on ecosystem functioning and its ecohydrological response to freeze-thaw cycles is seldomly reported. Here, the detailed vadose zone process model STEMMUS was coupled with the ecohydrological model T&C to investigate the role of solving the influential physical processes, considering different soil water and heat transfer parameterizations including frozen soils during freeze-thaw cycles. The physical representation is increased from using T&C without, and with the explicit consideration of ice effect to T&C coupling with STEMMUS enabling the simultaneous mass and energy transfer in the soil system (liquid, vapor, ice). We tested model performance with the aid of a comprehensive observation dataset collected at a typical meadow ecosystem on the Tibetan Plateau. Results indicated that: i) explicitly considering the frozen soil process significantly improved the soil moisture/temperature (SM/ST) profile simulations and facilitated our understanding of the water transfer processes within the soil-plant-atmosphere continuum; ii) the difference among various complexity representations of vadose zone physics have an impact on the vegetation dynamics mainly at the beginning of the growing season; iii) models with different vadose zone physics can predict similar interannual vegetation dynamics, and energy, water and carbon exchanges at the land-surface. This research highlights the important role of vadose zone models and their underlying physics, forin ecosystem functioning in cold regions and can guide support the development and applications of future earth Earth system models.

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1. Introduction

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Recent climatic changes have accelerated the dynamics of frozen soils in cold regions as for instance favoring permafrost thawing and degradation (Cheng and Wu, 2007; Hinzman et al., 2013; Peng et al., 2017; Yao et al., 2019; Zhao et al., 2019). In consequence of these changes, vegetation cover and phenology, land surface water and energy balances, subsurface soil hydrothermal regimes, water flow pathways were reported to be affected (Campbell and Laudon, 2019; Gao et al., 2018; Schuur et al., 2015; Walvoord and Kurylyk, 2016; Wang et al., 2012). Understanding how ecosystem functioning interacts with changing environmental conditions is a crucial yet challenging problem of earth-Earth system research for high latitude/altitude regions and deserves further attention. Various types of models, including

H_and surface models, terrestrial biosphere models, ecohydrology models, and hydrological models, have been widely utilized to enhance our knowledge in terms of land surface and processes, ecohydrological processes including the role of vegetation (Fatichi et al., 2016a;Fisher et al., 2014), and freezing/thawing process (Cuntz and Haverd, 2018;Druel et al., 2019;Ekici et al., 2014;Wang and Yang, 2018;Wang et al., 2017b). For instance, Zhuang et al. (Zhuang et al., 2001) incorporate a permafrost model into a large scale ecosystem model to investigate soil thermal temporal dynamics. Zhang et al. (Zhang et al., 2018) investigated the long term high-latitude Arctic tundra ecosystem response to the interannual variations of climate with the process based CoupModel. The LPJ-WHy model, with consideration of permafrost dynamics and peatland, was used to analyze land surface processes by (Wania et al., (2009). Lyu and Zhuang (Lyu and Zhuang, 2018) coupled a soil thermal model with the Terrestrial Ecosystem Model (TEM) to explore snowpack effects on soil thermal and carbon dynamics of the Arctic ecosystem under different climate scenarios.

A number of uncertainties are originated from different model structures. A more detailed knowledge of the effect of using a given model formulation can help toward making better projections of land surface dynamics, also in response to the call for joint efforts for systematic model developments (Clark et al., 2015; Yu et al., 2016). With emphasis on enhancing the underlying physics, most of the models have already adopted various solutions and parameterizations of land surface processes (e.g., Noah MP, CLM5, T&C) (Fatichi et al., 2012a, b; Niu et al., 2011; Lawrence et al., 2019), which facilitate the appropriate descriptions of different physical processes in various ecosystems. However, in most of the aforementioned these models, the water and heat transfer process in the vadose zone remains independent and not fully uncoupled, as they often adopt simplified approaches to water and heat transfer in the subsurface. Such physical parameterizations consideration of vadose zone physics might result in unsatisfactory simulations or unrealistic physical interpretations, especially when water and heat are tightly coupled as for instance in

freezing soilssoil freezing/thawing processes (Hansson et al., 2004). In this regard, researchers have stressed the necessity to simultaneously consider the water and heat transfer process in dry/cold seasons (Bittelli et al., 2008;Scanlon and Milly, 1994;Yu et al., 2016;Yu et al., 2018;Zeng et al., 2009a;Zeng et al., 2009b).

Concurrently, researchers developed dedicated models, e.g., SHAW (Flerchinger and Saxton, 1989), HYDRUS (Hansson et al., 2004), MarsFlo (Painter, 2011), and STEMMUS-FT (Yu et al., 2018), considering the soil water and heat coupling physics for frozen soils. Promising simulation results have been reported for the soil hydrothermal regimes. While these efforts mainly focus on understanding the surface and subsurface soil water and heat transfer process (Yu et al., 2018) and stress the role of physical representation of freezing/thawing process (Boone et al., 2000;Wang et al., 2017b;Zheng et al., 2017), they rarely take into account the interaction with vegetation and carbon dynamics.

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With the largest area of high-altitude permafrost and seasonally frozen ground, Tibetan Plateau is recognized as one of the most sensitive regions for climate change (Cheng and Wu, 2007; Liu and Chen, 2000; Yao et al., 2019). Monitoring and projecting the dynamics of hydrothermal and ecohydrological states and their responses to climate change in the Tibetan Plateau is considerably important to help shedding light on future ecosystem responses in this region. Considerable land-surface and vegetation changes have been reported in this region, e.g., degradation of permafrost and variations in seasonally frozen ground thickness changes of frozen ground (Cheng and Wu, 2007; Yao et al., 2019), advancing vegetation leaf onset dates (Zhang et al., 2013), and enhanced vegetation activity at the start of growing season (Qin et al., 2016). However, there are divergences with regard to the expected ecosystem modifications changes across the Tibetan Plateau (Cheng and Wu, 2007; Qin et al., 2016; Wang et al., 2018; Zhao et al., 2010)). (Zhao et al., 2010) (Wang et al., 2018) In response to climate warming, the degradation of frozen ground can positively affect the vegetation growth in Tibetan Plateau mountainous region (Qin et al., 2016), but it can also lead to degradation of grasslands (Cheng and Wu, 2007), depending on soil hydrothermal regimes and climate conditions (Qin et al., 2016; Wang et al., 2016). It is thus fundamental to have in situ multicomponent measurement networks (including meteorology, soil moisture/temperature, surface energy fluxes, carbon fluxes) to understand the environmental controls (Hao et al., 2011; Wang et al., 2017a; Wang et al., 2018; Zhao et al., 2010), validate terrestrial biosphere models and remote sensing products (He et al., 2014; Mwangi et al., 2020; Niu et al., 2016;Su et al., 2013;Tian et al., 2017), and extrapolate results via model data fusion methods to larger scales to better characterize land surface processes and ecosystem dynamics of the Tibetan Plateau (He et al., 2014; Zeng et al., 2016; Zhuang et al., 2020).

In this study, we <u>tested_investigated</u> the consequences of considering coupled water and heat transfer processes on land-surface fluxes and ecosystem dynamics in the extreme environmental conditions of the Tibetan plateau, relying on <u>the state-of-the-art land-surface</u> and ecohydrological <u>modeling-models</u> confronted with multiple field observations. The <u>limited knowledge of includingsion</u> or <u>not exclusion of complex different vadose zonesoil physical</u> processes, i.e., explicit considering ice effect and tightly coupled water and heat transfer, in such environment frames the scope here. Specifically, the driving questions of the research are: i) How <u>does</u> different <u>complexity in representing representations of frozen soil and coupled</u>

water and heat physics is affecting affect the simulated ecohydrological dynamics of a Tibetan plateau meadow? ii) How does model complexity different vadose zone physics affect our interpretation of mass, energy, and carbon fluxes at of the ecosystem scale? Answering these two questions is important to evaluate the adequacy of models to answer questions in understanding related ecosystem changes across the Tibetan Plateau.

In order to achieve the aforementioned goals, the detailed soil mass and energy transfer process developed in the STEMMUS model (Zeng et al., 2011a, b;Zeng and Su, 2013) was incorporated into the ecohydrology model Tethys-Chloris (T&C) (Fatichi et al., 2012a, b). The frozen soil physics was explicitly taken into account and soil water and heat transfer are-were fully coupled to further facilitating the model's capability in dealing with complex vadose zone processes.

2 Experimental Site and Data Methods

2.1 Experimental siteSite

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It is fundamental to have in situ multicomponent measurement networks (including meteorology, soil moisture/temperature, surface energy fluxes, carbon fluxes) to understand the environmental controls in ecosystem changes (Hao et al., 2011; Wang et al., 2017a; Wang et al., 2018; Zhao et al., 2010), to validate terrestrial biosphere models and remote sensing products (He et al., 2014; Mwangi et al., 2020; Niu et al., 2016; Su et al., 2013; Tian et al., 2017), and to extrapolate results via model-data-fusion to larger scales to better characterize land surface processes and ecosystem dynamics of the Tibetan Plateau (He et al., 2014; Zeng et al., 2016; Zhuang et al., 2020).

In this study, we make use of tThe Maqu soil moisture and soil temperature (SMST) monitoring network (Dente et al., 2012;Su et al., 2011;Su et al., 2013;Zeng et al., 2016), which is situated on the north-eastern fringe of the Tibetan Plateau. The monitoring network covers an area of approximately 40 km×80 km (33°30′–34°15′N, 101°38′–102°45′E) with the elevation varying from 3200 m to 4200 m above the sea level (a.s.l.). The climate can be characterized by wet rainy summers and cold dry winters. The mean annual air temperature (MAT) is 1.2°C with about -10.0°C and 11.7°C for the coldest month (January) and warmest month (July), respectively. The alpine meadows (e.g., *Cyperaceae* and *Gramineae*) dominate in this region with the a height of about 5 cm during the wintertime and 15 cm during the summertime. The general soil types are categorized as sandy loam, silt loam with a maximum of 18.3 % organic matter for the upper soil layers (Dente et al., 2012; Zhao et al., 2018; Zheng et al., 2015a; Zheng et al., 2015b). The groundwater level of the grassland area fluctuates from about 8.5 m to 12.0 m below the ground surface.

At For the Maqu SMST monitoring networksite, SMST profiles (5 cm, 10 cm, 20 cm, 40 cm, and 80 cm) are automatically measured by 5-TM ECH₂O probes (METER Group, Inc., USA) at a 15-min interval. The meteorological forcing (including wind speed/direction, air temperature and relative humidity at five heights above ground) is recorded by a 20 m Planetary Boundary Layer (PBL) tower system. An eddy-covariance system (EC150, Campbell Scientific, Inc., USA) was installed for monitoring the dynamics of the turbulent

heat fluxes and carbon fluxes. Instrumentations for measuring <u>four-four-component</u> down and upwelling solar and thermal radiation (NR01-L, Campbell Scientific, Inc., USA), and liquid precipitation (T200B, Geoner, Inc., USA) are also deployed.

For this research, data from March 2016 to August 2018 collected at the central experimental site (33°54′59″N, 102°09′32″, elevation: 3430m) were utilized (see Figure 1). Seasonally frozen ground is characteristic of this site, with the maximum freezing depth approaching around 0.8 m under current climate conditions. A few dedicated SMST profiles, with sensors installed at depths of 2.5 cm, 5 cm, 10 cm, 20 cm, 40 cm, 60 cm, and 100 cm, were used for validating the model simulations. Note that there are data gaps (25th Mar – 8th June, 2016; 29th Mar – 27th July, 2017, extended to 12th Aug, 2018 for 40 cm) due to the malfunction of instruments and the difficulty to maintain the network under such harsh environmental conditions. Furthermore, Wwe downloaded MCD15A3H (Myneni et al., 2015) and MOD17A2H (Running Steve et al., 2015) products for this site as the auxiliary representative of remotely sensed vegetation dynamics data from the Oak Ridge National Laboratory Distributed Active Center (ORNL DAAC) website. MCD15A3H provides an estimation of 8-day composites of LAI (Leaf Area Index) and FAPAR (Fraction of Absorbed Photosynthetically Active Radiation), while MOD17A2H an 8-day composite of GPP (Gross Primary Production (GPP)). Both MODIS products are at an aresolution of 500m.

2.2 Data

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Starting from the raw NEE (Net Ecosystem Exchange) and ancillary meteorological data (friction velocity u_* , global radiation R_g , soil temperature T_{soil} , air temperature T_{air} , and vapor pressure deficit VPD), we employed the REddyProc package (Reichstein et al., 2005; Wutzler et al., 2018) as a post-processing tool to obtain the time series of NEE, GPP (Gross Primary Production) and ecosystem respiration R_{eco} dynamics. Three different techniques, u_* filtering, gap filling, and flux partitioning, were adopted in REddyProc package. The periods with low turbulent mixing is firstly determined and filtered for quality control (u_* filtering, (Papale et al., 2006)). Then, the marginal distribution sampling (MDS) algorithm was used as the gap_filling method to replace the missing data (Reichstein et al., 2005). Finally, NEE was separated into GPP and R_{eco} by night-time based and day-time based approaches (Lasslop et al., 2010).

170 2.3-2.2 Precipitation, evapotranspiration Evapotranspiration, and frost Frost front Front

The observed surface water conditions over the entire study period, including the precipitation and cumulative evapotranspiration (which is obtained by summing up the hourly latent heat flux measured by EC system), are shown in Figure: +2a. Both ET and precipitation are low until the end of the freezing period (see Figure: +2b), during this early period the daily average ET is 0.15 mm/d. During the growing season, the

cumulative precipitation increases and ET follows with a lower magnitude a lower rate. The average daily ET for the entire observation period is 1.45 mm/d.

Figure 42b presents the development of freezing depth with time (the freezing depth development of the year 2017-2018 was incomplete due to the absence of soil temperature data). Several freezing/thawing cycles frequently occurred at the beginning of the winter, which initializes the Freezing-Thawing (FT) process. Frost The freezing front starts-started to propagate with a rate of 1.34 cm/d, reaching its maximum depth at around 80cm for the year 2016-2017. Then the thawing process is was activated by the atmospheric forcing at the surface and subsurface soil heat flux, acting at the from the soil surface and bottom of the soil, respectively.

2.43 Modelling the soilSoil-plantPlant-atmosphere Atmosphere continuumContinuum

2.43.1 Overview of Tethys-Chloris T&C Model (unCPLD)

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The Tethys-Chloris model (T&C) (Fatichi et al., 2012b) simulates the coupled-dynamics of energy, water, and vegetation and has been successfully applied to a very large spectrum of ecosystems and environmental conditions as summarized elsewhere (Fatichi and Ivanov, 2014; Fatichi et al., 2016b; Fatichi and Pappas, 2017; Mastrotheodoros et al., 2017; Pappas et al., 2016). The model simulates the energy, water, and carbon exchanges between the land surface and the atmospheric surface layer accounting for aerodynamic, undercanopy, and leaf boundary layer resistances, as well as for stomatal and soil resistance. The model further describes vegetation physiological processes including photosynthesis, phenology, carbon allocation, and tissue turnover. Dynamics of water content in the soil profile in the plot-scale version are solved using the one-dimensional (1-D) Richards equation. Heat transfer in the soil is solved by means of the heat diffusion equation. Soil heat and water dynamics are uncoupled (however, note that T&C is termed unCPLD to distinguish it later with the coupling with STEMMUS). A-The detailed model description is provided in the above-mentioned references and some key elements applied for this article-study are discussed explained in the following.

<u>T&C</u> model uses the 1-D Richards equation, which describes the water flow under gravity and capillary forces in isothermal conditions, is solved in T&C for variably saturated soils:

$$\rho_L \frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} - S = \rho_L \frac{\partial}{\partial z} \left[K \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] - S \tag{1}$$

where θ (m³ m³) is the volumetric water content; q (kg m² s¹) is the water flux; z (m) is the vertical direction coordinate; S (kg m³ s¹) is the sink term for transpiration and evaporation fluxes. ρ_L (kg m³) is the liquid water density; K (m s¹) is the soil hydraulic conductivity; ψ (m) is the soil water potential; t (s) is the time. In T&C, the nonlinear partial differential equation is solved using a finite volume approach with the method of lines (MOL) (Lee et al., 2004). MOL discretizes the spatial domain and reduces the partial differential equation to a system of ordinary differential equations in time, which can be expressed as:

$$d_{z,i}\frac{d\theta_i}{dt} = q_{i-1} - q_i - T_v r_{v,i} - E_s - E_{bare}$$
(2)

where $d_{z,i}$ (m) is the thickness of layer i; q_i (m s⁻¹) is the vertical outflow from a layer i; T_y (m s⁻¹) is the transpiration fluxes from the vegetation; $r_{v,i}$ is the fraction of root biomass contained in soil layer i; E_{bare} (m s⁻¹), evaporation from the bare soil; E_s (m s⁻¹), evaporation from soil under the canopy.

The heat conservation equation used in the T&C neglects the coupling of water and heat transfer physics and only the heat conduction component is considered, which can be expressed as:

$$\rho_{soil}C_{soil}\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\lambda_{eff}\frac{\partial T}{\partial z}\right) \tag{3}$$

where ρ_{soil} (kg m⁻³) is the bulk soil density; C_{soil} (J kg⁻¹ K⁻¹) is the specific heat capacities of bulk soil; λ_{eff} (W m⁻¹ K⁻¹) is the effective thermal conductivity of the soil. T (K) is the soil temperature. When soil undergoes freezing/thawing process, the latent heat due to water phase change becomes important, which is not considered in the original T&C model, but it is in the T&C-FT (freezing/thawing) model.

215 <u>3.2 T&C-FT Model (unCPLD-FT)</u>

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To account for frozen soil, T&C-FT model considers ice effect on hydraulic conductivity, thermal conductivity, heat capacity, and subsurface latent heat flux. However, the vapor flow and the thermal effect on water flow are not considered in T&C-FT, and during the non-frozen period, soil water and heat are still independently transferred as in T&C (this version is named here unCPLD-FT). To explicitly account for freezing/thawing processes, the heat conservation equation is written as:

$$\rho_{soil}C_{soil}\frac{\partial T}{\partial t} - \rho_{ice}L_f\frac{\partial \theta_{ice}}{\partial t} = \frac{\partial}{\partial z}\left(\lambda_{eff}\frac{\partial T}{\partial z}\right) \tag{4}$$

where the latent heat associated with the freezing/thawing process is explicitly considered and ice water content θ_{ice} is a prognostic variable, which is simulated along with liquid water content for each soil layer. Specifically, when Eq. (4) is rewritten in terms of an apparent volumetric heat capacity C_{app} (Gouttevin et al., 2012;Hansson et al., 2004), it can be solved equivalently to Eq. (3):

$$C_{app} \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\lambda_{eff} \frac{\partial T}{\partial z} \right) \tag{5}$$

where C_{app} can be computed knowing the temperature T (K), latent heat of fusion L_f and the differential (specific) water capacity $d\theta/d\psi$ at a given liquid water content θ (Hansson et al., 2004):

$$C_{app} = \rho_{soil}C_{soil} + \rho_{ice}\frac{L_f^2}{gT}\frac{d\theta}{d\psi}$$
 (6)

The effective thermal conductivity λ_{eff} (W m⁻¹ K⁻¹) and the specific soil heat capacity C_{soil} (J kg⁻¹ K⁻¹) are computed accounting for solid particles, water, and ice content (Farouki, 1981;Johansen, 1975;Lawrence et al., 2018;Yu et al., 2018). The soil freezing characteristic curve providing the liquid water potential in a frozen soil is computed following the energy conservative solution proposed by Dall'Amico et al. (2011) and it can be combined with various soil hydraulic parameterizations including van-Genuchten and Saxton and Rawls to compute the maximum liquid water content at a given temperature and consequently ice and liquid content profiles at any time step (Fuchs et al., 1978;Yu et al., 2018).

Finally, saturated hydraulic conductivity is corrected in the presence of ice content (e.g., (Hansson et al., 2004; Yu et al., 2018)). Note, that beyond latent heat associated with phase change and changes in thermal and hydraulic parameters because of ice presence, all the other soil physics processes described by STEMMUS are not considered here, and heat and water fluxes are still not entirely coupled in T&C-FT.

2.4.23.3 Overview of STEMMUS Model

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STEMMUS (Simultaneous Transfer of Energy, Mass and Momentum in Unsaturated Soil) model solves soil water-movement, soil air flow, and soil heat flow balance equations simultaneously in one timestep (Zeng et al., 2011a, b;Zeng and Su, 2013). The Richards' equation with modifications made by Milly (Milly, 1982) was is utilized to mimic the coupled soil mass and energy transfer process. The dry air is considered to be an independent phase in the soil. The vapor diffusion, advection, and dispersion are all taken into account as the water vapor transport mechanisms. In addition to the soil moisture and temperature gradient, the atmospheric pressure gradient acts as the third driving force for soil water, vapor and heat flow. RThe root water uptake process is regarded as the sink term of soil water and heat balance equations, building up the linkage between soil and atmosphere (Yu et al., 2016). In STEMMUS, temporal dynamics of three phases of water (liquid, vapor and ice) are explicitly presented and simultaneously solved by spatially discretizing the corresponding governing equations of liquid water flow and vapor flow.

$$\frac{\partial}{\partial t} (\rho_L \theta_L + \rho_V \theta_V + \rho_{ice} \theta_{ice}) = -\frac{\partial}{\partial z} (q_{Lh} + q_{LT} + q_{Vh} + q_{VT}) - S$$

$$= \rho_L \frac{\partial}{\partial z} \left[K \left(\frac{\partial \psi}{\partial z} + 1 \right) + D_{TD} \frac{\partial T}{\partial z} \right] + \frac{\partial}{\partial z} \left[D_{Vh} \frac{\partial \psi}{\partial z} + D_{VT} \frac{\partial T}{\partial z} \right] - S$$
(7)

where ρ_V and ρ_{ice} (kg m⁻³) are the density of water vapor and ice, respectively; θ_L , θ_V and θ_{ice} (m³ m⁻³) are the soil liquid, vapor and ice volumetric water content, respectively; q_{Lh} and q_{LT} (kg m⁻² s⁻¹) are the soil liquid water flow driven by the gradient of soil matric potential $\frac{\partial \psi}{\partial z}$ and temperature $\frac{\partial T}{\partial z}$, respectively. q_{Vh} and q_{VT} (kg m⁻² s⁻¹) are the soil water vapor fluxes driven by the gradient of soil matric potential $\frac{\partial \psi}{\partial z}$ and temperature $\frac{\partial T}{\partial z}$, respectively. D_{TD} (kg m⁻¹ s⁻¹ K⁻¹) is the transport coefficient of the adsorbed liquid flow due to temperature gradient; D_{Vh} (kg m⁻² s⁻¹) is the isothermal vapor conductivity; and D_{VT} (kg m⁻¹ s⁻¹ K⁻¹) is the thermal vapor diffusion coefficient.

STEMMUS takes into account different heat transfer mechanisms, including heat conduction (λ_{eff} $\frac{\partial T}{\partial z}$), convective heat transferred by liquid and vapor flow, the latent heat of vaporization ($\rho_V \theta_V L_0$), the latent heat of freezing/thawing ($-\rho_{ice}\theta_{ice}L_f$) and a source term associated with the exothermic process of wetting of a

porous medium (integral heat of wetting) $(-\rho_L W \frac{\partial \theta_L}{\partial t})$.

$$\frac{\partial}{\partial t} \left[(\rho_S \theta_S C_S + \rho_L \theta_L C_L + \rho_V \theta_V C_V + \rho_{ice} \theta_{ice} C_{ice}) (T - T_{ref}) + \rho_V \theta_V L_0 - \rho_{ice} \theta_{ice} L_f \right] - \rho_L W \frac{\partial \theta_L}{\partial t}$$

$$= \frac{\partial}{\partial z} \left(\lambda_{eff} \frac{\partial T}{\partial z} \right) - \frac{\partial}{\partial z} \left[q_L C_L (T - T_{ref}) + q_V (L_0 + C_V (T - T_{ref})) \right] - C_L S (T - T_{ref})$$
(8)

where ρ_s (kg m⁻³) is the soil solids density; θ_s is the volumetric fraction of solids in the soil; C_s , C_L , C_V and C_{ice} (J kg⁻¹ K⁻¹) are the specific heat capacities of soil solids, liquid, water vapor and ice, respectively; T_{ref} (K) is the arbitrary reference temperature; L_0 (J kg⁻¹) is the latent heat of vaporization of water at the reference temperature; L_f (J kg⁻¹) is the latent heat of fusion; W (J kg⁻¹) is the differential heat of wetting (expressed by Edlefsen and Anderson (1943) as the amount of heat released when a small amount of free water is added to the soil matrix). q_L and q_V (kg m⁻² s⁻¹) are the liquid and vapor water flux, respectively. Additional details on the equations for solving the coupled water and heat equations can be found in Zeng et al. (2011a, b) and Zeng and Su (2013). In the appendix, a notation table is summarized for the above equations.

3.4 Coupling T&C and STEMMUS (CPLD)

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As mentioned above (section 3.1-3.2), T&C considers soil water and heat dynamics independently, and T&C-FT only considers ice effects associated with latent heat, thermal and hydraulic parameters, while all other soil physics processes of STEMMUS are not considered. On the other hand, while STEMMUS model can well reproduce the soil water and heat transfer process in frozen soil, it lacks a detailed description of land-surface processes and of the ecohydrological feedback mechanisms. To take advantage of the strengths of both models, we coupled STEMMUS model with the land-surface and vegetation components of T&C model (termed as CPLD) to better describe the soil-plant-atmosphere continuum (SPAC) in cold regions.

The current coupling procedure between STEMMUS and the T&C model is based on a sequential coupling via exchanging mutual information within one timestep (see Figure 3). T&C model and STEMMUS model run sequentially within one timestep. First, the preparation and initialization modules are called. Meteorology inputs and constant parameters are set, and the initialization process is performed. After the inputs are prepared, the main iteration process starts. T&C is in charge of the time control information (starting time, time step, elapsed time) and informs STEMMUS model with these time settings every time step. Meanwhile, the surface boundary conditions obtained by the solution of vegetation and land-surface energy dynamics are also sent to drive STEMMUS model. The surface latent heat flux (LE) is partitioned into soil evaporation (used for setting the surface boundary condition of soil water flow) and plant transpiration (further subdivided into layer-specific root water uptakes representing the sink terms of Richard equation).

After convergence is achieved in the soil module (i.e., convergence criteria is set as 0.001 for both soil matric potential [in cm] and soil temperature [in K]), STEMMUS estimates soil temperature/soil moisture (hereafter as ST/SM) profiles, which are utilized to update ST/SM states in T&C model. T&C model then utilizes these updated ST/SM information (rather than its own computed ST/SM profiles) to proceed with the ecohydrological simulations in the following time step. Such iteration continues till the end of simulation period.

3.5 Numerical Experiments

To investigate the role of increasing complexity of vadose zone physics in ecosystem functioning, three numerical experiments were designed on the basis of the aforementioned modeling framework (Table 1). First experiment, the T&C original model was run as stand-alone, termed as unCPLD simulation. For the unCPLD model, soil water and heat transfer is independent with no explicit consideration of soil ice effect. The second experiment, the updated T&C model with explicit consideration of freezing/thawing process was run as it can estimate the dynamics of soil ice content and the related effect on water and heat transfer (e.g., blocking effect on water flow, heat release/gain due to phase change) but otherwise being exactly equal to T&C original model. This second simulation is named the unCPLD-FT simulation, where the term unCPLD generally refers to the fact that T&C model and STEMMUS model are not yet coupled. The third experiment, STEMMUS model was coupled with T&C model to enable not only frozen soil physics but also additional processes and most importantly the tight coupling of water and heat effects. This simulation is named CPLD simulation. In this third scenario, vapor flow, which links the soil water and heat flow, is explicitly considered. In addition to the ice blocking effect as presented in unCPLD-FT, the thermal effect on water flow is also expressed with the temperature dependence of hydraulic conductivity and matric potential. Furthermore, not only the latent heat due to phase change, but also the convective heat due to liquid/vapor flow is simulated.

Hourly meteorological forcing (including downwelling solar radiation, precipitation, air temperature, relative humidity, wind speed, atmospheric pressure) was utilized to drive the models. For the adaptive time step of STEMMUS simulation, linear interpolation between two adjacent hourly meteorological measurements was used to generate the required second values. The hydrological related initial states, e.g., initial snow water equivalent, soil water and temperature profiles, were taken as close as possible to the observed ones. Since the current initial conditions of the carbon and nutrients pools in the soil are unknown, we spin-up carbon and nutrient pools running only the soil-biogeochemistry module for 1000 years using average climatic conditions and prescribed litter inputs taken from preliminary simulations. Then we used the spun-up pools as initial conditions for the hourly-scale simulation over the period for which hourly observations are available. This last operation is repeated two times which allows reaching a dynamic equilibrium of nutrient and carbon pools in the soil and vegetation.

The total depth of soil column was set as 3m and divided into 18 layers with a finer discretization in the upper soil layers (1-5cm) than that in the lower soil layers (10-50cm). Soil samples were collected and transported to the laboratory to determine the soil hydrothermal properties (see Zhao et al., (Zhao et al., 2018) for detail). The average soil texture and fitted Van Genuchten parameters at three soil layers were listed in supplement Table S1. Vegetation parameters were obtained on the basis of literature and expert knowledge (see a summary of the adopted vegetation parameters in the supplement Table S2). All three numerical experiments shared the same soil and vegetation parameter settings.

2.4.3 Difference between STEMMUS and T&C models in mass and energy transfer process

While T&C model specializes in dealing with the interaction between vegetation and the hydrological system, it simplified the soil water and heat transfer process in the hydrology component, e.g., ignored water vapor flow, dry air flow, and, in the original version, does not contain freezing/thawing process, as water is always in liquid phase regardless of sub-zero soil temperatures. To extend the application of T&C model over frozen soil, a freeze thaw module has been incorporated for this study as described below. Furthermore, while STEMMUS model can well reproduce the soil water and heat transfer process, it lacks detailed description of land-surface processes and of the vegetation-hydrology feedback mechanisms. To take advantage of the strengths of both models, we coupled STEMMUS with the land surface and vegetation components of T&C model to better describe the soil plant atmosphere continuum.

1) Mass transfer process

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The 1-D Richards equation, which describes the water flow under gravity and capillary forces in isothermal conditions, is solved in T&C for variably saturated soils.

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial x} - S = \rho_L \frac{\partial}{\partial x} \left[K \left(\frac{\partial \psi}{\partial x} + 1 \right) \right] - S \tag{1}$$

where $\theta(m^3 m^{-3})$ is the volumetric water content; q (kg m⁻² s⁻¹) is the water flux; z (m) is the vertical direction coordinate; S (s⁻¹) is the sink term for transpiration, evaporation and lateral transfer fluxes. ρ_L (kg m⁻³) is the liquid water density; K (m s⁻¹) is the soil hydraulic conductivity; ψ (m) is the soil water potential; t (s) is the time.

In T&C, the nonlinear partial differential equation is solved using a finite volume approach with the method of lines (MOL) (Lee et al., 2004). MOL discretizes the spatial domain and reduces the partial differential equation to a series of ordinary differential equations in terms of time, which can be expressed as

$$\frac{d\theta_{t}}{dt} = q_{t-1} - q_{t} - \left(\sum_{j=1}^{n_{c}} T_{H_{v,l,j}} r_{H_{v,l,j}}\right) - \left(\sum_{j=1}^{n_{c}} T_{L_{v,l,j}} r_{L_{v,l,j}}\right) - \left(\sum_{j=1}^{n_{c}} E_{s,j}\right) - E_{pare} + Q_{t,in,t}$$

$$\frac{-Q_{t,v,t,j}}{2} - \frac{Q_{t,v,t,j}}{2} - \frac{Q_{t,v,t,j}}$$

where q_t (m s⁻¹) is the vertical outflow from a layer i, T_{Hv} , and T_{Lv} (m s⁻¹) are the transpiration fluxes from the high—and low vegetation layers, respectively. E_{bare} (m s⁻¹), evaporation from the bare soil. E_s (m s⁻¹), evaporation from soil under the eanopy. $Q_{t,in,t}$, $Q_{t,out,t}$ (m s⁻¹)—are the incoming lateral subsurface fluxes and lateral outflows, respectively. (Gouttevin et al., 2012;Hansson et al., 2004)(Hansson et al., 2004)(Farouki, 1981;Johansen, 1975;Lawrence et al., 2018;Yu et al., 2018)(Dall'Amico et al., 2011)(Fuchs et al., 1978;Yu et al., 2018)(Hansson et al., 2004;Yu et al., 2018)

While in STEMMUS, temporal dynamics of three phases of water (liquid, vapor and ice), together with the soil dry air component, are explicitly presented and simultaneously solved by spatially discretizing the corresponding governing equations of liquid water flow, vapor flow and dry air flow.

$$\frac{\partial}{\partial t} (\rho_L \theta_L + \rho_V \theta_V + \rho_I \theta_{ICC}) = -\frac{\partial}{\partial z} (q_{Lh} + q_{LT} + q_{La} + q_{Vh} + q_{VT} + q_{Va}) - S$$

$$= \rho_L \frac{\partial}{\partial z} \left[K \left(\frac{\partial \psi}{\partial z} + 1 \right) + D_{TD} \frac{\partial T}{\partial z} + \frac{K}{\gamma_W} \frac{\partial P_g}{\partial z} \right] + \frac{\partial}{\partial z} \left[D_{Vh} \frac{\partial \psi}{\partial z} + D_{VT} \frac{\partial T}{\partial z} + D_{Va} \frac{\partial P_g}{\partial z} \right] - S$$
(3)

where ρ_V and ρ_i (kg m⁻³) are the density of water vapor and ice, respectively; $\theta_{L\tau}$, θ_V and θ_{ice} (m³ m⁻³) are the soil liquid, vapor and ice volumetric water content, respectively; q_{LR} , q_{LR} , and q_{LR} (kg m⁻²-s⁻¹) are the soil liquid water flow driven by the gradient of soil matric potential $\frac{\partial \psi}{\partial z}$, temperature $\frac{\partial T}{\partial z}$, and air pressure $\frac{\partial P_H}{\partial z}$, respectively. q_{VR} , q_{VR} , and q_{VR} (kg m⁻²-s⁻¹) are the soil water vapor fluxes driven by the gradient of soil matric potential $\frac{\partial \psi}{\partial z}$, temperature $\frac{\partial T}{\partial z}$, and air pressure $\frac{\partial P_H}{\partial z}$, respectively. T (°C) is the soil temperature; and P_S (Pa) is the mixed pore air pressure. γ_{WC} (kg m⁻²-s⁻²) is the specific weight of water. D_{TD} (kg m⁻¹-s⁻¹-°C⁻¹) is the transport coefficient of the adsorbed liquid flow due to temperature gradient; D_{VH} (kg m⁻²-s⁻¹) is the isothermal vapor conductivity; and D_{VT} (kg m⁻¹-s⁻¹-°C⁻¹) is the thermal vapor diffusion coefficient; D_{VR} is the advective vapor transfer coefficient. (Zeng et al., 2011a, b)(Zeng and Su, 2013)

2) Energy transfer process

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The heat conservation equation used in the original T&C neglects the coupling of water and heat transfer physics and only the heat conduction component is considered, which can be expressed as below

$$C_{soil} \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\lambda_{eff} \frac{\partial T}{\partial z} \right) \tag{4}$$

where C_{soit} (J kg⁻¹ °C⁻¹) is the specific heat capacities of bulk soil; λ_{eff} (W m⁻¹ °C⁻¹) is the effective thermal conductivity of the soil. When soil undergoes freezing/thawing process, the latent heat due to water phase change becomes important but is not included in the original T&C model.

STEMMUS takes into account different heat transfer mechanisms, including heat conduction $(\lambda_{eff} \frac{\partial F}{\partial z})$, convective heat transferred by liquid, vapor and air flow, the latent heat of vaporization $(\rho_V \theta_V L_0)$, the latent heat of freezing/thawing $(-\rho_t \theta_t L_F)$ and a source term associated with the exothermic process of wetting of a porous medium (integral heat of wetting) $(-\rho_L W \frac{\partial \theta_L}{\partial z})$.

$$\frac{\partial}{\partial t} \left[(\rho_{S} \theta_{S} C_{S} + \rho_{L} \theta_{L} C_{L} + \rho_{V} \theta_{V} C_{V} + \rho_{dd} \theta_{a} C_{a} + \rho_{l} \theta_{l} C_{l}) (T - T_{r}) + \rho_{V} \theta_{V} L_{0} - \rho_{l} \theta_{l} L_{f} \right] - \rho_{L} W \frac{\partial \theta_{L}}{\partial t}$$

$$= \frac{\partial}{\partial z} \left(\lambda_{eff} \frac{\partial T}{\partial z} \right) - \frac{\partial}{\partial z} \left[q_{L} C_{L} (T - T_{r}) + q_{V} (L_{0} + C_{V} (T - T_{r})) + q_{a} C_{a} (T - T_{r}) \right] - C_{L} S (T - T_{r}) \tag{5}$$

where ρ_s (kg m⁻³) is the soil solids density; θ_s is the volumetric fraction of solids in the soil; C_s , C_L , C_V , C_a and C_r (J kg⁻¹ °C⁻¹) are the specific heat capacities of soil solids, liquid, water vapor, dry air and ice, respectively; T_r (°C) is the arbitrary reference temperature; L_0 (J kg⁻¹) is the latent heat of vaporization of water at the reference temperature; L_f (J kg⁻¹) is the latent heat of fusion; W (J kg⁻¹) is the differential heat of wetting (expressed by Edlefsen and Anderson (1943) as the amount of heat released when a small amount of free water is added to the soil matrix). q_{L_f} q_{V_f} and q_a (kg m⁻² s⁻¹) are the liquid, vapor water flux and air flow, respectively. Additional details and the air flow balance equation for solving the coupled water and heat equations can be found in Zeng et al. (2011a, b) and Zeng and Su (2013).

2.4.4 T&C model with freezing/thawing process

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In the T&C version modified to explicitly account for freezing/thawing processes, the heat conservation equation is written as:

$$C_{soil} \frac{\partial T}{\partial t} - \rho_t L_f \frac{\partial \theta_t}{\partial t} = \frac{\partial}{\partial z} \left(\lambda_{eff} \frac{\partial T}{\partial z} \right) \tag{6}$$

where the latent heat associated with the freezing/thawing process is explicitly considered and ice water content θ_i is a prognostic variable, which is simulated along with liquid water content for each soil layer. Specifically, when Eq. (7) is rewritten in terms of an apparent specific heat capacity C_{app} (Gouttevin et al., 2012; Hansson et al., 2004) it can be solved equivalently to Eq. (4):

$$C_{app} \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\lambda_{eff} \frac{\partial T}{\partial z} \right) \tag{7}$$

where C_{app} can be computed knowing the temperature T, latent heat of fusion L_f and the differential (specific) water capacity $d\theta/d\psi$ at a given water content (Hansson et al., 2004):

$$C_{app} = C_{soit} + \rho_i \frac{L_T^2}{gT} \frac{d\theta}{d\psi}$$
(8)

The effective thermal conductivity λ_{eff} (W m⁻¹ °C⁻¹) and the specific soil heat capacity C_{soil} (J kg⁻¹ °C⁻¹) are computed accounting for solid particles, water, and ice content (Farouki, 1981;Johansen, 1975;Yu et al., 2018;Lawrence et al., 2018). The soil freezing characteristic curve providing the maximum liquid water content at a given temperature is computed following Dall'Amico et al. (2011) and it can be combined with various soil hydraulic parameterization including van Genuchten, Clapp and Hornberger and Saxton and Rawls (Fuchs et al., 1978;Yu et al., 2018).

Finally, saturated hydraulic conductivity is corrected in presence of ice content (e.g., (Hansson et al., 2004;Yu et al., 2018)). Note, that beyond latent heat associated with phase change and changes in thermal and hydraulic parameters because of ice presence, all the other soil physics processes described by STEMMUS are neglected and heat and water fluxes are still uncoupled in this version of T&C.

2.5 Coupling procedure

The current coupling procedure between STEMMUS and the original T&C is based on a sequential coupling via exchanging mutual information within one timestep (see Figure 2). T&C model and STEMMUS model ran sequentially within one timestep. First, the preparation and initialization module are called. Meteorology inputs and constant parameters are set, and the initialization process is performed. After the input are prepared, the main iteration process starts. T&C is in charge of the time control information (starting time, time step, elapsed time) and informs STEMMUS model with these time settings every time step. Meanwhile, the surface boundary conditions obtained by the solution of vegetation and land surface energy dynamics are also sent to drive STEMMUS model. The surface latent heat flux (LE) is partitioned into soil evaporation (used for setting the surface boundary condition of soil water flow) and plant transpiration (further subdivided into layer specific root water uptakes representing the sink terms of Richard equation). After convergence

achieves in the soil module, STEMMUS estimates soil temperature/soil moisture (hereafter as ST/SM) profiles, which are utilized to update ST/SM states in T&C model. T&C model then utilizes these updated ST/SM information (rather than its own computed ST/SM profiles) to proceed with the ecohydrological simulations in the following time step. Such iteration continues till the end of simulation period.

2.6 Design of numerical experiment

To investigate the role of increasing complexity of vadose zone physics in ecosystem functioning, three numerical experiments were designed on the basis of aforementioned modeling framework. First experiment, the T&C original model was ran as stand alone, termed as unCPLD simulation. Second experiment, the updated T&C model with explicit consideration of freezing/thawing process is run as it can estimate the dynamics of soil ice content and the related effect on water and heat transfer (e.g., blocking effect on water flow, heat release/gain due to phase change) but otherwise being exactly equal to T&C original model. This second simulation is named the unCPLD FT simulation. Third experiment, STEMMUS model was coupled with T&C model to enable one to consider not only a simplified frozen soil physics but also additional processes and most important water and heat effects are tightly coupled and affect each other. This simulation is named—CPLD simulation.

All three numerical experiments shared the same soil and vegetation parameter settings to accommodate the conditions of a Tibetan meadow. The total depth of soil column was set as 3m and divided into 18 layers with a finer discretization in the upper soil layers (1 5cm) than that in the lower soil layers (10 50cm). Soil samples were collected and transported to the laboratory to determine the soil hydrothermal properties (see Zhao et al. (2018) for detail). The average soil texture and fitted Van Genuchten parameters at three soil layers were listed in supplement Table S1. Vegetation parameters were obtained on the basis of physical constraints, literature, and expert knowledge (see a summary of the adopted vegetation parameters in the supplement Table S2).

4. Results and Discussion

3 Results

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34.1 Surface fluxes Fluxes simulations Simulations

The 5-day moving average dynamics of the net incoming radiation (Rn), latent heat (LE) and sensible heat (H) fluxes measured and simulated by the unCPLD model, unCPLD-FT₂ and CPLD model for the study period are presented (Figure 34). The seasonality and magnitude of surface fluxes can be captured across seasons. A good match between observed and simulated Rn and LE was identified during the whole period, with isolated observable discrepancies (Fig.-ure 34a & c and Figure S1). Compared with unCPLD and unCPLD-FT simulations, CPLD model simulated the similar dynamics of LE while generally produced a

larger overestimation of *Rn*, especially during the frozen period. These mismatches of *Rn* can be partly attributed to the uncertainties of observed winter precipitation events and the following snow cover dynamics, which might not be well captured in the models; because the true winter precipitation is difficult to observe. For the sensible heat flux simulations, all three models can reproduce the seasonal dynamics. However, an overestimation of the 5-day average values was observed in several periods. Given the good correspondence between observations and simulations of net radiation and latent heat, this discrepancy might be a model shortcoming due to the simplification of considering only one single surface prognostic temperature (i.e. soil surface and vegetation surface temperature were assumed the same), but it can be also generated caused by the lack of energy balance closure in the flux towereddy-covariance data (see Sect. 4.14.5). Compared with unCPLD and unCPLD-FT simulations, the overestimation was however reduced by in the CPLD model simulations and the *H* dynamics was closer to the observations during the growing season.

The correlation between observed and simulated <u>daily average</u> surface heat fluxes with unCPLD, unCPLD-FT, and CPLD model is shown in Figure- 45 and Figure S2-3. Noticeably all the unCPLD/CPLD model scenarios, with different water and heat transfer physics, exhibited nearly identical statistical performance of surface fluxes simulations (Fig-ure 45). There is an overestimation of *H* reproduced by three model simulations. The CPLD model presented less overestimation of *H* compared to unCPLD models. The overall performance of the model in terms of turbulent flux simulations could be regarded as acceptable given current uncertainties in winter precipitation and <u>flux towereddy-covariance</u> observations in such a challenging environment, even though discrepancies exist during certain periods (Fig-ure 34).

34.2 Soil moisture Moisture and Soil Temperature sSimulations

The capability of the three models to reproduce the temporal dynamics of soil moisture is illustrated in Figure 56. By explicitly considering soil ice content, the unCPLD-FT and CPLD model captured well the response of soil moisture dynamics to the freezing/thawing processfreeze-thaw cycles.— Wwhile the unCPLD model lacks-lacked such capability and maintains-maintained a higher soil moisturewater content throughout the winter period, which then reflect inbut slightly lower water contents in the growing season. For all three models, the consistency between the measured and model simulated soil water content at five soil layers is was satisfactory during the growing season, indicating the models' capability in portraying the effect of precipitation and root water uptake on the soil moisture conditions.

3.3 Soil temperature simulations

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Five layers of soil temperature measurements were employed to test the performance of the model in reproducing the soil thermal regimetemperature profiles (Fig.ure 76). During the growing period, all three models can well-capture well the dynamics of soil temperature at various depth with fluctuating atmospheric forcing. In this period, there is no significant difference among the three models with regards to about the magnitude and temporal dynamics of soil temperature. During the freezing period, a general underestimation of soil temperature and overestimation of its diurnal fluctuations were found at shallower soil layers, which

may indicate that there is some thermal buffering effect in reality not fully considered captured in the models. Compared with unCPLD-FT and CPLD models, the unCPLD model simulations have had stronger diurnal fluctuations of soil temperature with an underestimation of temperature at the beginning of the freezing period and a considerable overestimation during the thawing phase. This results in an earlier date passing the 0°C threshold than in the unCPLD-FT and CPLD simulations. It should be noted that for the deeper soil layers (e.g., 60cm in Figure 7), all models tended to simulate the early start of freezing soil temperatures and considerably underestimated the soil temperature during the frozen period. This can be due to the uncertainties in soil organic layer parameters, the not fully captured snow cover effect (Gouttevin et al., 2012), a potentially pronounced (Gouttevin et al., 2012) heterogeneity in soil hydrothermal properties, or the potential role of solutes on the freezing-point depression (the presence of solute lowers the freezing soil temperature) (Painter and Karra, 2014). These mismatches in deep soil temperature degraded the model performance in simulating the dynamics of liquid water (Figure 6) and ice content (Figure 8) during the frozen period.

3.44.3 Soil ice-Ice content Content and water-Water fluxFlux

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The simulated time-series of soil ice content and water flux from both-unCPLD, unCPLD-FT and CPLD model simulations for soil layers below 2 cm are presented in Figure 78. As soil ice content measurements were not available, the freezing front propagation inferred from the soil temperature measurements was employed to qualitatively testify assess the model performance. The phenomenon that a certain amount of liquid water flux moves upwards along with the freezing front can be clearly noticed for both the unCPLD-FT and CPLD model simulations. As the soil matric potential changes sharply during the water phase change, a certain amount of water fluxes will be forced towards the phase changing region, a phenomenon known as cryosuction. Such a phenomenon has already been demonstrated from theoretical and experimental perspectives by many researchers (Hansson et al., 2004; Watanabe et al., 2011; Yu et al., 2018). Cryoscution is much more accentuated in the unCPLD-FT simulation, while it is of course absent in the unCPLD model simulations (Figure 8c). Precipitation induced downward water flux can be observed in all models during summer and they are very similar. It is to note that compared to unCPLD-FT model, CPLD model presented a relatively lower presence of soil ice content, while its temporal dynamics was closer to the observed freezing/thawing front propagation. The difference between the two simulations can be attributed to the constraints imposed by the interdependence of liquid, ice, and vapor in the soil pores that is considered only in CPLD model, A deeper presence of soil ice content was reproduced by the unCPLD FT model, as indicated by a deeper freezing front propagation than the in situ measurements. CPLD model presented a relative good match of soil freezing dynamics as it is physically constrained by the inter-dependence of liquid, ice, vapor, air components in soil pores. The phenomenon that a certain amount of liquid water flux moves upwards along with the freezing front can be clearly noticed from the unCPLD FT and CPLD model simulations. As the soil matric potential changes sharply during the water phase change period, a certain amount of water fluxes will be forced towards the phase changing region, a phenomenon known as cryosuction. Such a

phenomenon has already been demonstrated from theoretical and experimental perspectives by many researchers (Hansson et al., 2004; Watanabe et al., 2011; Yu et al., 2018). This is of course absent from the unCPLD model simulations (Fig. 7c). Nevertheless, the precipitation induced downward water flux can be observed in both models.

3.54.4 Simulations of land-Land surface Surface carbon-Carbon fluxesFluxes

The eddy covariance derived <u>vegetation productivity</u> and remote sensing (MODIS) observations of vegetation dynamics are compared with the model simulation in Fig-ure 89. When compared with in situ <u>flux-towereddy-covariance</u> observations, a-slightly earlier growth and considerably earlier senescence of grassland with lower photosynthesis <u>was-were</u> inferred from MODIS *GPP* product (Figure- 98a). The mismatch in the phenology <u>are is</u> likely a combined issue of 8-day (or longer if clouds are impeding the view) composite of MODIS products and challenge of translating vegetation reflectance signals into productivity or Leaf Area Index (LAI) during the grass senescent phase.

Trusting Taking the temporal dynamics of flux towereddy-covariance observations as the reference, the onset date of grassland appears to be well captured by both unCPLD and CPLD model simulations, while a delayed onset date is reproduced by unCPLD-FT model. Leaf senescence and dormancy phase are a bit delayed in the models when compared with flux-towereddy-covariance data and considerably delayed when compared to MODIS-LAI, even though the latter is particularly uncertain as described above. Although there is an observable underestimation of GPP compared to the eddy covariance measurements, the dynamics of GPP, which is mainly constrained by the photosynthetic activity and environmental stresses, is reasonably reproduced by all model simulations.

The underestimation of GPP has magnified consequences in terms of reproducing *NEE* dynamics by unCPLD/CPLD models. While this might be seen as a model shortcoming, there are a number of reasons that lead to questioning the reliability of the magnitude of carbon fluxes measurements at this site. By checking other ecosystem productivity under similar conditions, the annual average *GPP* for the Tibetan plateau meadow ecosystem ranges from 300 to 935 g C m⁻² yr⁻¹, while the annual average *NEE* ranges from -79 to -213 g C m⁻² yr⁻¹ (see the literature summary in the Supplement Table \$2\$3). While the EC system used in this experimental site observes an annual *GPP* and *NEE* as 1132.52 and -293.24 g C m⁻² yr⁻¹. Both the *GPP* and *NEE* measured fluxes are significantly larger than previous existing estimates of the carbon exchange for such a type of ecosystem type (and representative of much more productive ecosystems) and are unlikely to be correct in absolute magnitude. The ecosystem respiration (R_{eco}), indicating the respiration of activity of all living organisms in an ecosystem is shown in Fig-ure \$9d. The performance of all three model simulations in reproducing R_{eco} dynamics can be characterized as an overall good match with regards to the magnitude and seasonal dynamics of R_{eco} , which further suggests the discrepancy in observed/simulated *GPP* is the driver of the discrepancy disagreement inof *NEE*.

The difference in the soil liquid water/temperature profile simulations between the CPLD and unCPLD models (as shown in Fig-ure 56 & 67) resulted in differences in simulated vegetation dynamics, especially concerning the leaf onset date, which is affected by integrated winter soil temperatures. The unCPLD-FT model has a delay in the vegetation onset date when compared to the other simulations, due to the significant cryosuction that prolongs freezing conditions and keep lower soil temperatures. This makes the unCPLD simulations have having a slightly lower-shorter vegetation activity active season compared to the CPLD model simulations. The lower GPP in the unCPLD simulations is instead related to either because of a delayed leaf onset (unCPLD FT) or because of a slightly enhanced water-stress (unCPLD) induced by the different soil-moisture dynamics during the winter and summer season. Indeed, there is with a slight-lower root zone moisture produced by the unCPLD model (Fig-ure 56), which affects the plant photosynthesis and growth, thus the vegetation dynamics in T&C. Differences in soil temperature profiles can also affect root respiration ingenerating additional small differences in GPP. The unCPLD FT model has a delay in the vegetation onset date, due to its prolonged freezing conditions as derived from soil temperature simulations than the other simulations.

4 Discussion

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44.5.1 Surface energy Energy balance Balance elosure Closure

The energy balance closure problem, usually identified because the sum of latent (LE) and sensible (H) heat fluxes is less than the available energy (Rn- G_0), is quite common in eddy covariance measurements (Leuning et al., 2012; Wilson et al., 2002). The energy imbalance of EC measurements is particularly significant at the sites over the Tibetan Plateau (Tanaka et al., 2003; Yang et al., 2004; Chen et al., 2013; Zheng et al., 2014). Figure 9-10 presents the energy balance imbalance of hourly LE and H by the eddy covariance measurements, observed Rn by the four-component radiation measurements, and the estimated ground heat flux (G_0) by CPLD model. The sum of measured LE and H was significantly less than Rn, with the slope of LE+H versus Rn equal to 0.59 (Figure, 910a). Usually, the measurements of radiation are reliable (Yang et al., 2004). If we assume that the turbulence fluxes (LE, H) measurements were are accurate, then the rest of energy (around 41% of Rn) should be theoretically consumed by ground heat flux G_0 , which is clearly impossible. When compared to the available energy (Rn- G_0), the slope was increased to 0.70 (Figure, 910b). Table 1-2 further demonstrated that the energy imbalance problem was significant across all seasons. The seasonal variation of energy closure ratio (ECR) can be identified for the case LE+H versus Rn- G_0 , similar to the research of Tanaka et al., 2003), i.e., a good energy closure during the pre-monsoon periods while a degraded one during the summer monsoon periods.

These problems are clearly suggesting that care should be taken in the model to data comparison, but they are not affecting the comparison among models with different complexity vadose zone physics as we did not

force any parameter calibration or data-fitting procedure, but simply rely on physical constraints, literature, and expert knowledge to assign model parameters.

44.6.2 Effects on water Water budget Budget components Components

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The effect of different model scenarios on soil water budget components is illustrated in Figure- 10. T&C model can describe in details the different water budget components. Precipitation can be partitioned into vegetation interception, surface runoff, and infiltration. Infiltrated water can then be used for surface evaporation (Es), root water extraction (transpiration, Tv), and changes in soil water storage (ΔVs). The other evaporation components, i.e., evaporation from intercepted canopy water (E_{IN}) and snow cover (E_{SN}), can be further distinguished by T&C model. A certain amount of water will drain below the bottom of the 3 m soil column as deep leakage (L_K).

All model eases demonstrated that most of the precipitation is used by ET. Compared to the unCPLD case, Less amount of water was consumed by ET according to from unCPLD-FT simulations than that from unCPLD. This is due to the less-lower amount of vegetation transpiration (Tv) and intercepted canopy water evaporation (E_{IN}) amount because of cooler late winter temperatures and the late beginning of the active vegetation season. The cooler late winter temperatures from unCPLD-FT simulations can be attributed to the retardation of the thawing process due to the phase change-induced heat absorption and the soil ice-induced modification of bulk heat capacity during the freezing-thawing transition period, which damped the magnitude of temperature variations and delayed the thawing process. This explains the higher value of Δ Vs for unCPLD FT simulation (5.22%) than that of unCPLD simulation (2.88%). With explicit consideration of soil ice, hydraulic conductivity is also reduced and vertical water flow is retarded during the frozen period (Kurylyk and Watanabe, 2013). This explains the higher value of ΔVs of unCPLD-FT simulation (5.2%) than that of unCPLD simulation (2.8%). However Furthermore, at the end of the freezing period, the unCPLD-FT simulation presents a delayed vegetation onset thus a decrease of ecosystem water consumption, which favors percolation toward deeper layers and the bottom leakage. Such a positive effect on the bottom leakage flux was slightly weaker than the negative effect (impeded water flow) due to frozen soil throughout the winter season. These results indicate that the presence of seasonally frozen soil can mediate the water storage in the vadose zone via both hydrological and plant physiological controls.

The effect of coupled water and heat physics (unCPLD v₇s. CPLD model) on the water budget components can be summarized as: i) the amount of ecosystem water consumption ET was reduced, due to the damped surface evaporation process (evaporation from the soil surface and intercepted water). ii) water storage amount in the vadose zone increased while the bottom leakage decreased. We attribute this to the way ice content is simulated in the CPLD simulation, and also to the temperature dependence of soil hydraulic conductivity (see Table 1 and Supplement S1). Specifically, the high accumulation of ice content in the unCPLD-FT simulations indicates a relatively stronger cryosuction effect than in CPLD simulations. This cryosuction effect is mitigated in the fully coupled model because of water vapor transfer and thermal gradients, even though different solutions in the parameterization of bulk soil thermal conductivity and

volumetric soil heat capacity could also be responsible for the difference. Overall, T taking into account the fully coupled water and heat physics modifies the temporal dynamics of ice formation and thawing in the soil and activates temperature effects on water flow (i.e., low soil temperature will slow down water movement). That implies that soil water flow toward and at the bottom soil layer is retarded when coupled water and heat physics is considered (as reflected by less leakage water flux for CPLD simulations).

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Given the same atmospheric forcing and the same model structure to represent land-surface exchanges and vegetation dynamics, how water/heat transfer processes are represented in the soildifferent vadose zone physics generates differences in SM and ST vertical profiles. From the perspective of energy and carbon fluxes, the convective heat flux and explicit frozen soil physics are taken into account in the CPLD model while they are not considered in the two unCPLD models. The liquid water flux-induced convective heat flux is mostly relevant during the frozen period (Boike et al., 2008; Kane et al., 2001; Yu et al., 2020). As it has been observed, a certain amount of liquid water/vapor flux moves toward the freezing front and this effect is different between unCPLD-FT and CPLD while absent in unCPLD (Figure 8). For the unfrozen period, instead, the total mass fluxes were comparable between the two unCPLD and CPLD simulations. For the temperature gradient, there is not much difference between unCPLD and CPLD simulations during both the growing season and frozen period. The liquid water flux induced convective heat flux is mostly relevant during the frozen period(Boike et al., 2008; Kane et al., 2001). As it has been observed, a certain amount of liquid water/vapor flux moving toward the freezing front (Fig. 7), resulting in a convective heat toward the front. Such amount of The heat convection and mostly the heat release by freezing and consumed by the melting processes slows down the freezing/thawing process and decreases the diurnal and seasonal temperature fluctuations (Figure, 56). Different soil thermal profiles have consequences on the vegetation dynamic process (Figure, 99), mainly by modifying the temperature profile in the soil, which affects the beginning of the growing season and the subsequent simulated photosynthesis and growth processes. This is consistent with the decadal observation results of Li et al. (Li et al., 2016), in which they reported the cumulative temperature effect on the carbon dynamics as it breaks the vegetation dormancy, affects the leaf phenology and plant growth dynamics. From the perspective of water fluxes, it is during the frozen period that water and heat transfer processes are tightly coupled (Hansson et al., 2004; Yu et al., 2018). Both the explicit consideration of soil ice and coupled water and heat physics can affect the vadose zone water flow via altering the hydraulic conductivity. This is testified by the fact that even the unCPLD-FT simulation accounting for soil-freezing in a simplified way in comparison to STEMMUS (e.g., the CPLD simulation) cannot recover the exact same dynamics of ice content (Fig.ure 78), which impacts leaf onset and to a less extent hydrological fluxes. (Jiang et al., 2012; Wang et al., 2012) However, in the rest of the year, the simplified solution of vadose zone physics of T&C leads to very similar results as the coupled one, suggesting

that most of the additional physics does not modify substantially the ecohydrological response <u>during</u> <u>unfrozen periods</u>.

5-6 Conclusion

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The detailed vadose zone process model STEMMUS and the ecohydrological model T&C were coupled to investigate the effect of various model complexities representations in simulating water and energy transfer and seasonal ecohydrological dynamics over a typical Tibetan meadow. The results indicate that the original T&C model tended to overestimate the variability and magnitude of soil temperature during the freezing period and the freezing-thawing transition period. Such mismatches were ameliorated by the inclusion of soil ice content and freezing-thawing to the original model and further improved by the model with explicit consideration of soil ice content dynamics and coupled water and heat physics. For the largest part of the simulated period (i.e., unfrozen), we found that a simplified treatment of vadose zone dynamics is sufficient to reproduce satisfactory energy, water and carbon fluxes – given the uncertainty in the flux-towereddycovariance observations. Additional complexity in vadose zone representation is mostly significant during the freezing and thawing periods as ice content simulations differs among models and a certain the amount of water moving towards the freezing front was mostly differently reproduced simulated by the coupled model while it cannot be simulated by the original model and the modified model cannot account for the heat associated with this water movement. These differences discrepencies have an impact (even though limited to the beginning of the growing season) on vegetation dynamics. The leaf onset is better captured by the unCPLD and CPLD models, while a delayed onset date was reproduced by unCPLD-FT model. Nonetheless, overall patterns for the rest of the year do not differ considerably among simulations, which suggest that vadose zone dynamics with a fully coupled water-heat model treatment are not different enough to affect the overall ecosystem response. This also suggests that the additional complexity might be more needed for specific vadose zone studies and investigation of permafrost thawing rather than for ecohydrological applications. In summary, our investigations using different models of vadose zone physics could be helpful to guide support the development and applications of future earth system models applications as they suggest that a certain degree of complexity might be necessary only in specific analyses.

Data availability. The soil hydraulic/thermal property data can be accessed from 4TU. Center for Research Data (https://doi.org/10.4121/uuid:61db65b1-b2aa-4ada-b41e-61ef70e57e4a). The other relevant data are available from https://doi.org/10.6084/m9.figshare.12058038.v1 or from Data Archiving and Networked Services (DANS) https://easy.dans.knaw.nl/ui/datasets/id/easy-dataset:160877 upon registration.

Author contribution. Conceptualization, Z.S. and Y.Z.; methodology, L.Y., Y.Z., and S.F.; writing - original draft preparation, L.Y., Y.Z., S.F., Z.S.; writing - review & editing, L.Y., Y.Z., S.F., Z.S.

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

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Notation

Symbol	<u>Parameter</u>	<u>Unit</u>
$\underline{C_{app}}$	Apparent heat capacity	$J kg^{-1} K^{-1}$
$\underline{C_{ice}}$	Specific heat capacity of ice	$J kg^{-1} K^{-1}$
<u>C</u> L	Specific heat capacity of liquid	$\frac{\text{J kg}^{-1} \text{ K}^{-1}}{\text{I}}$
\underline{C}_s	Specific heat capacity of soil solids	$\frac{\text{J kg}^{-1} \text{ K}^{-1}}{\text{I}}$
<u>Csoil</u>	Specific heat capacity of the bulk soil	$\frac{\text{J kg}^{-1} \text{ K}^{-1}}{\text{I}}$
\underline{C}_{V}	Specific heat capacity of water vapor	$\frac{\text{J kg}^{-1} \text{ K}^{-1}}{\text{I}}$
$d_{z,i}$	Thickness of layer i	<u>m</u>
\underline{D}_{Vh}	Isothermal vapor conductivity	$kg m^{-2} s^{-1}$
\underline{D}_{VT}	Thermal vapor diffusion coefficient	kg m ⁻¹ s ⁻¹ K ⁻¹
\underline{D}_{TD}	Transport coefficient for adsorbed liquid flow due to temperature gradient	kg m ⁻¹ s ⁻¹ K ⁻¹
\underline{E}_{bare}	Evaporation from the bare soil	$\underline{\mathbf{m}} \ \mathbf{s}^{-1}$
\underline{E}_s	Evaporation from soil under the canopy	<u>m s⁻¹</u>
<u>K</u>	Hydraulic conductivity	<u>m s⁻¹</u>
<u>K</u> s	Soil saturated hydraulic conductivity	<u>m s⁻¹</u>
$\underline{L}_{\!f}$	<u>Latent heat of fusion</u>	$J kg^{-1}$
\underline{L}_0	Latent heat of vaporization of water at the reference temperature	<u>J kg⁻¹</u>
<u>n</u>	Van Genuchten fitting parameters	Ξ
<u>q</u>	Water flux	kg m ⁻² s ⁻¹
q_i	Vertical outflow from a layer i	m s ⁻¹
<u>q</u> L	Soil liquid water fluxes (positive upwards)	$kg m^{-2} s^{-1}$
<u>qv</u>	Soil water vapor fluxes (positive upwards)	$kg m^{-2} s^{-1}$
q_{Lh}	Liquid water flux driven by the gradient of matric potential	kg m ⁻² s ⁻¹
$q_{\scriptscriptstyle LT}$	Liquid water flux driven by the gradient of temperature	kg m ⁻² s ⁻¹
q_{Vh}	Water vapor flux driven by the gradient of matric potential	kg m ⁻² s ⁻¹
q_{VT}	Water vapor flux driven by the gradient of temperature	kg m ⁻² s ⁻¹
$r_{v,i}$	Fraction of root biomass contained in soil layer i	Ξ
<u>S</u>	Sink term for transpiration, evaporation	$kg m^{-3} s^{-1}$
<u>t</u>	<u>Time</u>	<u>s</u>
<u>T</u>	Soil temperature	<u>K</u>
$\underline{T_{ref}}$	Arbitrary reference temperature	<u>K</u>
$\underline{T}_{\underline{v}}$	<u>Transpiration fluxes from the vegetation</u>	<u>m s⁻¹</u>
\underline{W}	Differential heat of wetting	$J kg^{-1}$
<u>z</u>	Vertical space coordinate (positive upwards)	<u>m</u>
α	Air entry value of soil	<u>m⁻¹</u>
ψ	Water potential	<u>m</u>
λ_{eff}	Effective thermal conductivity of the soil	${ m W} { m m}^{-1} { m K}^{-1}$
<u> Qice</u>	Density of ice	$kg m^{-3}$
<u>P</u> L	Density of soil liquid water	kg m ⁻³
<u> </u>	Bulk soil density	$\frac{1}{\text{kg m}^{-3}}$
<u> </u>	Density of solids	$\frac{1}{\text{kg m}^{-3}}$
<u> </u>	Density of water vapor	$\frac{1}{\text{kg m}^{-3}}$
<u> </u>	Volumetric water content	$m^3 m^{-3}$

$\underline{ heta}_{ice}$	Soil ice volumetric water content	$m^{3} m^{-3}$
$\underline{\theta_L}$	Soil liquid volumetric water content	$\underline{\mathrm{m}^3 \ \mathrm{m}^{-3}}$
$\underline{\theta}_{\mathrm{r}}$	Residual soil water content	$\underline{\mathrm{m}^3 \ \mathrm{m}^{-3}}$
$\underline{\theta_{s}}$	Volumetric fraction of solids in the soil	$\underline{\mathrm{m}^3 \ \mathrm{m}^{-3}}$
$\underline{ heta}_{ ext{sat}}$	Saturated soil water content	$\underline{\mathrm{m}^3 \mathrm{m}^{-3}}$
<u>\theta_V</u>	Soil vapor volumetric water content	$\underline{\text{m}^3 \text{ m}^{-3}}$

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Tables and Figures

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Table 1. Numerical experiments with various mass and energy transfer processes

E	Soil Physical Processes	<u>S</u>	Model Components	
Experiments	<u>Unfrozen period</u>	Frozen period		
unCPLD	independent WHT	independent WHT; no ice effect; no LH due to phase change	T&C (Eqs. 1 & 3)	
unCPLD-FT	independent WHT	FT induced WHT coupling; ice effect; LH due to phase change	T&C-FT (Eqs. 1 & 4)	
<u>CPLD</u>	tightly coupled WHT	tightly coupled WHT; ice effect; LH due to phase change; CH due to liquid/yapor flow	T&C-STEMMUS (Eqs. 7 & 8)	

Note: Independent WHT, Soil Water and Heat Transfer process is independent.

FT induced WHT coupling, Soil Water and Heat Transfer process is coupled only during the freezing/thawing (FT) period. Soil water flow is affected by temperature due to the temperature dependency of hydraulic conductivity (the impedance effect as the presence of soil ice content).

Tightly coupled WHT, Soil Water and Heat Transfer process is tightly coupled; vapor flow, which links the soil water and heat flow, is taken into account; thermal effect on water flow is considered (the hydraulic conductivity and matric potential is dependent on soil temperature; when soil freezes, the hydraulic conductivity is reduced by the presence of soil ice, which is temperature dependent); the convective/advective heat due to liquid/vapor flow can be calculated. Ice effect, the explicit simulation of ice content and its effect on the hydraulic/thermal properties.

LH due to phase change, latent heat due to the phase change.

CH due to liquid/vapor flow, convective heat due to liquid/vapor flow.

 $1|150 \qquad \text{Table $\frac{12}{2}$. Monthly values of energy closure ratio derived from eddy covariance measured LE+H versus Rn and Rn-G_0, respectively (Dec. 2017-Aug. 2018). G_0, the ground heat flux, was estimated by CPLD model.}$

Energy closure ratio	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug
(LE+H) vs Rn	0.58	0.58	0.61	0.45	0.53	0.55	0.55	0.57	0.59
$(LE+H)$ vs $(Rn-G_0)$	0.98	0.90	0.90	0.51	0.62	0.68	0.64	0.63	0.67

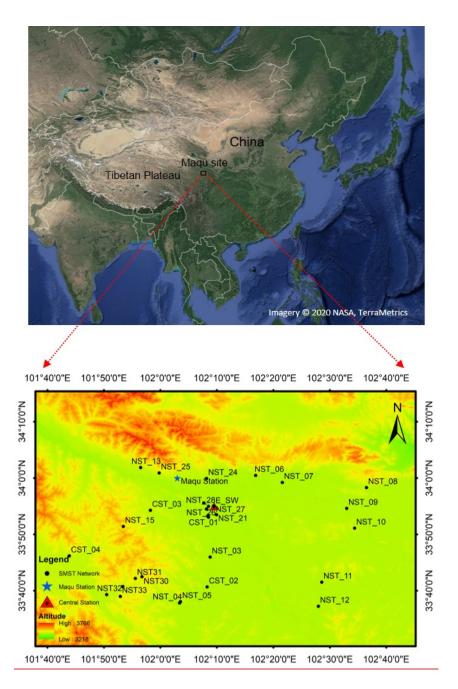
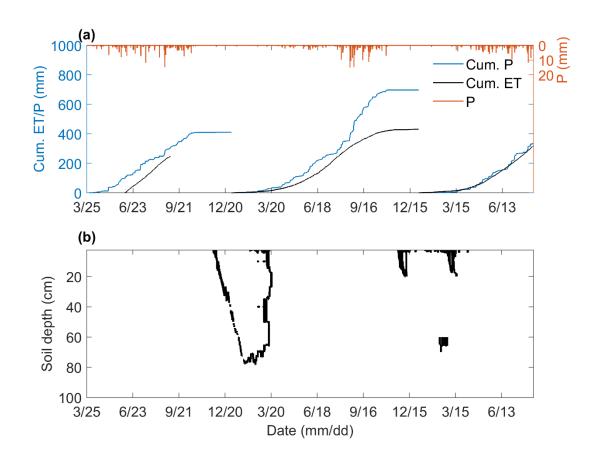


Figure 1. Geographical location of Maqu soil moisture/temperature (SMST) monitoring network and the Centre station.



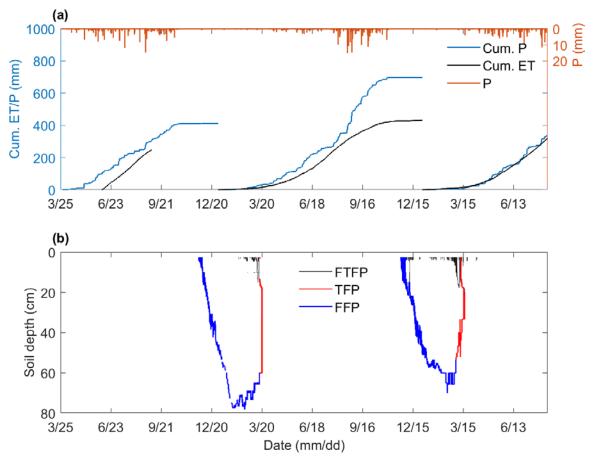


Figure 42. Observed cumulative precipitation (P) and evapotranspiration (ET) (a) and observed propagation of freezing/thawing front (FTFP), with the blue and red color for the propagation of freezing front and thawing front (FFP & TFP), respectively (b) for the period 25 Mar. 2016- 12 Aug. 2018 at Maqu site.

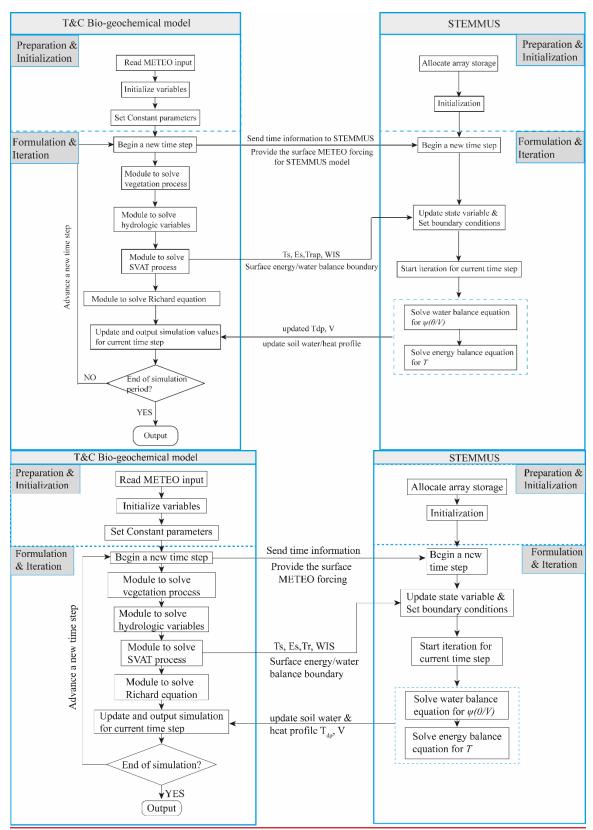
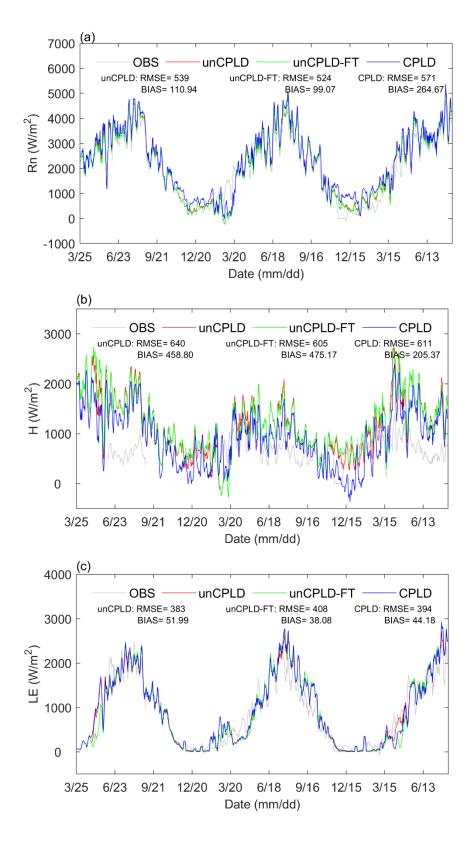


Figure 23. Coupling procedure of STEMMUS and T&C model. METEO is the meteorology forcing, SVAT is acronym for the Soil-Vegetation-Atmosphere mass and heat Transfer. Ts, Es, Trap, WIS are the surface



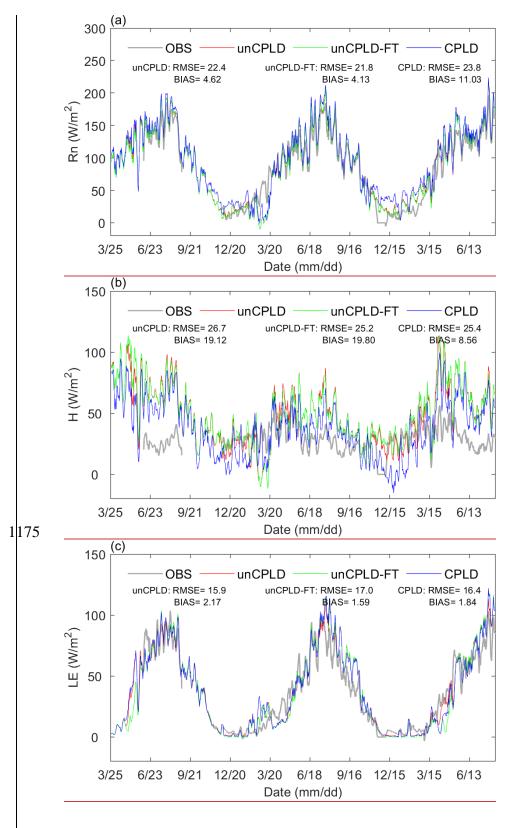
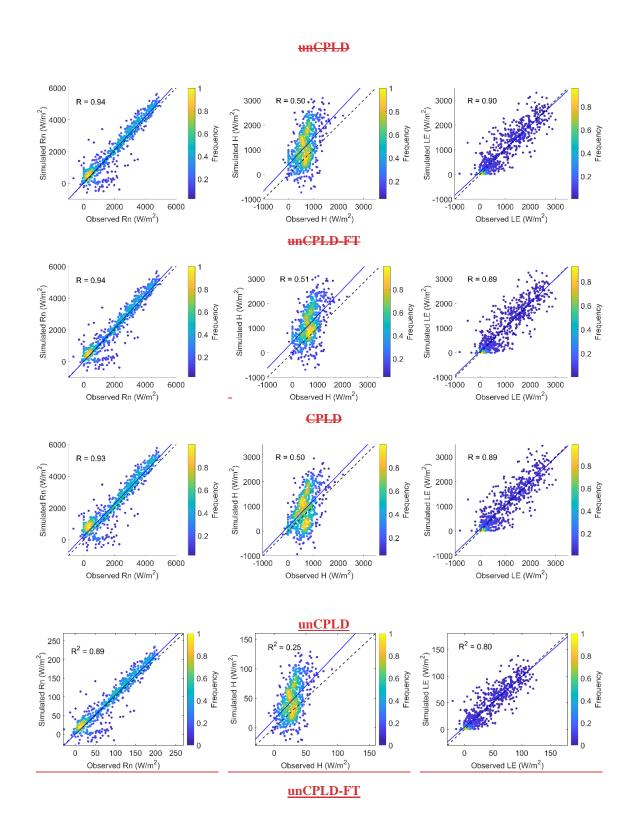


Figure 34. Comparison of observed and simulated 5-day moving average dynamics of net radiation_(Rn), latent heat flux_(LE), and sensible heat flux_(H) using the original (uncoupled) T&C (unCPLD), T&C with consideration of FT process (unCPLD-FT) and coupled T&C and STEMMUS (CPLD) model.



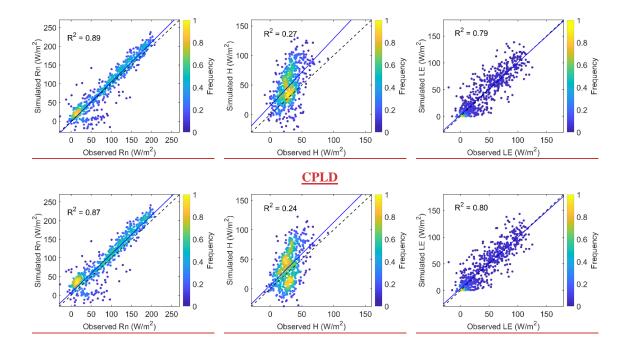


Figure 45. Scatter plots of observed and model simulated daily average surface fluxes (net radiation: Rn, latent heat: LE and sensible heat flux: H) using the original (uncoupled) T&C (unCPLD), T&C with consideration of FT process (unCPLD-FT) and coupled T&C and STEMMUS (CPLD) model, with the color indicating the occurrence frequency of surface flux values.

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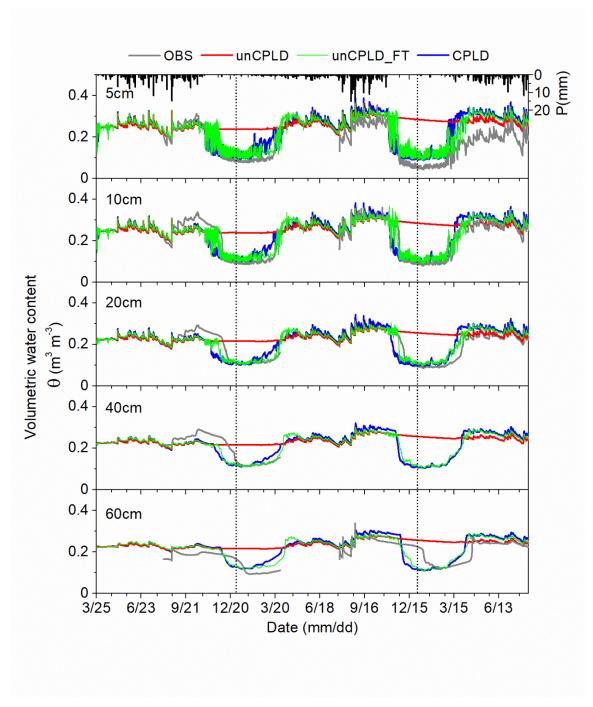
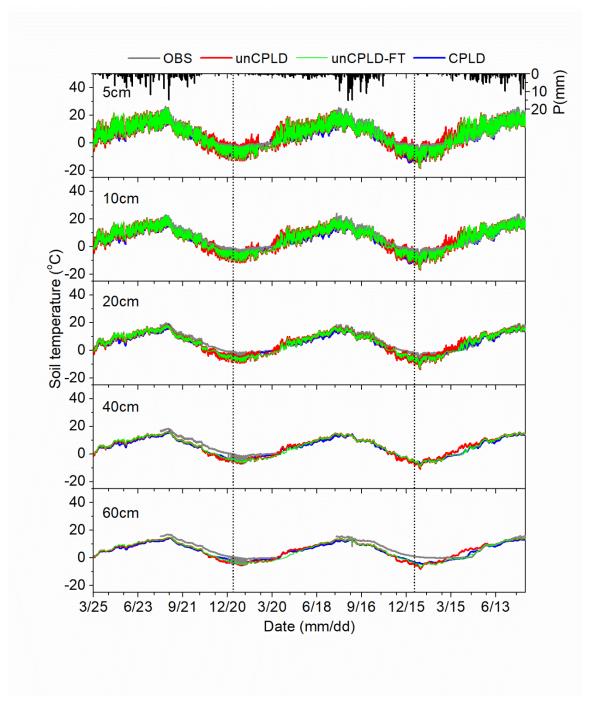
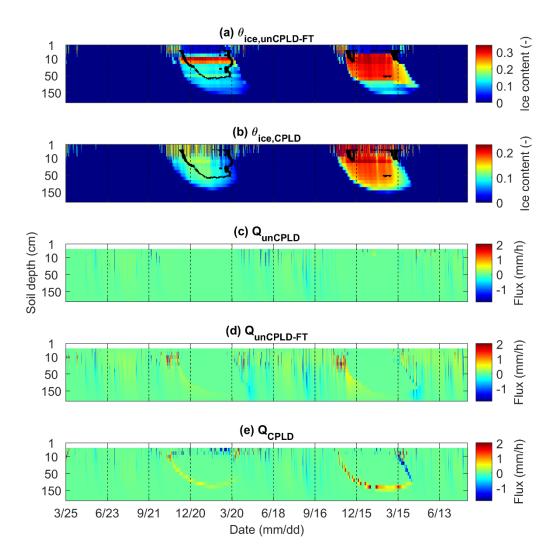


Figure 56. Measured and estimated soil moisture at various soil layers using uncoupled T&C (unCPLD), uncoupled T&C with FT process (unCPLD-FT) and coupled T&C and STEMMUS (CPLD) model. Note that in unCPLD model, soil ice content is not explicitly considered, thus all the water remains in a liquid phase, which is leading to a strong overestimation of winter soil water content in frozen soils.



 $[1200] Figure \ \hbox{$67$.} \ Measured and simulated soil temperature at various soil layers using uncoupled T\&C (unCPLD), T\&C with FT process (unCPLD-FT) and coupled T\&C and STEMMUS (CPLD) model.$



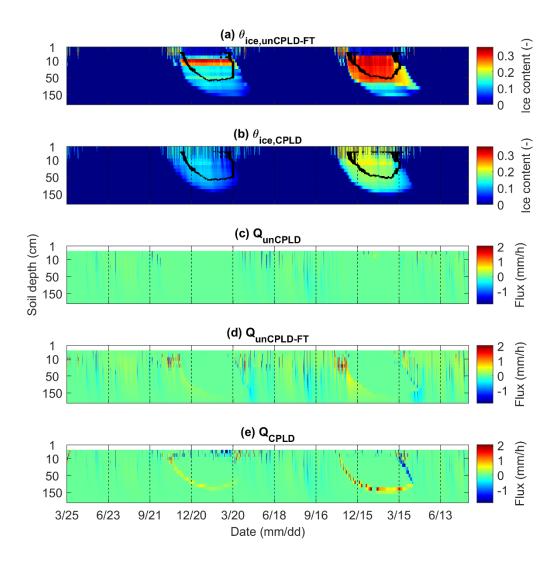
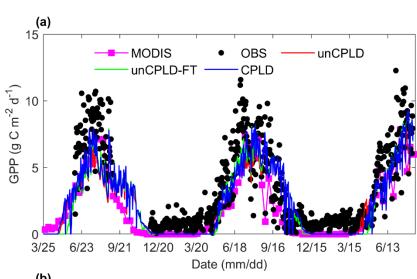
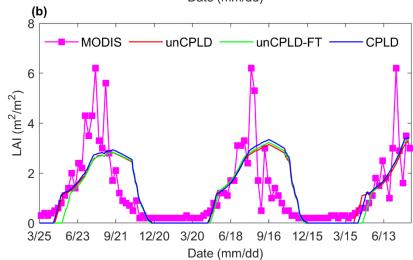


Figure 78. Soil ice content from (a) unCPLD-FT and (b) CPLD model simulations with freezing front propagation derived from the measured soil temperature and vertical water flux from (c) unCPLD, (d) unCPLD-FT and (e) CPLD model simulations, not temperature and vertical water flux from (c) unCPLD model and the fluxes of top 1-2 cm soil layers were erased not reported to highlight fluxes of the lower layers.





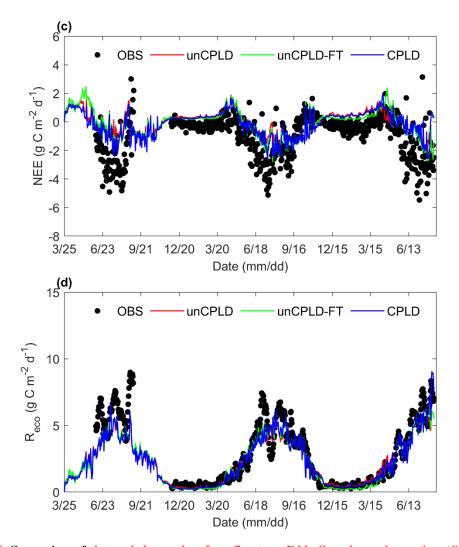


Figure 89. Comparison of observed observations from flux-towerEddy Covariance observations (OBS) or MODIS remote sensing and simulated (a) Gross Primary Production (GPP), (b) Leaf Area Index (LAI), (c) Net Ecosystem Exchange (NEE), and (d) Ecosystem respiration (Recor) using unCPLD, unCPLD-FT, and CPLD model. MODIS refers to the data from MODIS-GPP and MODIS-LAI products.

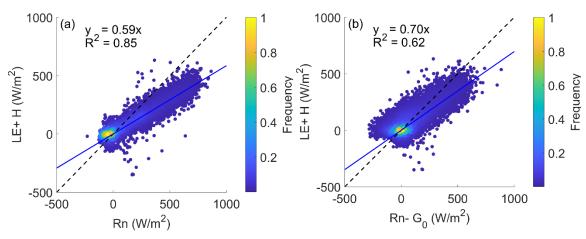
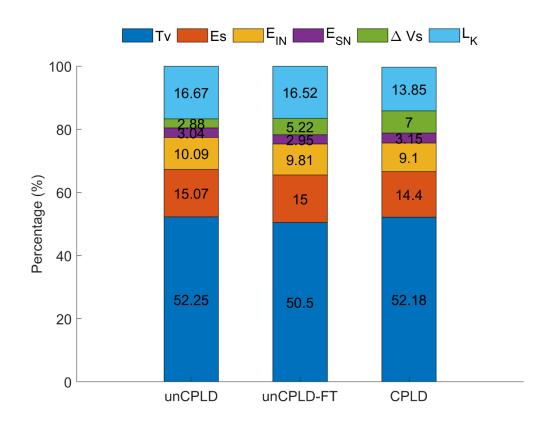


Figure 910. Scatter plots of eddy covariance measured hourly values of LE + H versus (a) Rn and (b) Rn-G₀, with the color indicating the occurrence frequency of surface flux values. G_0 , the ground heat flux, was estimated by the CPLD model.



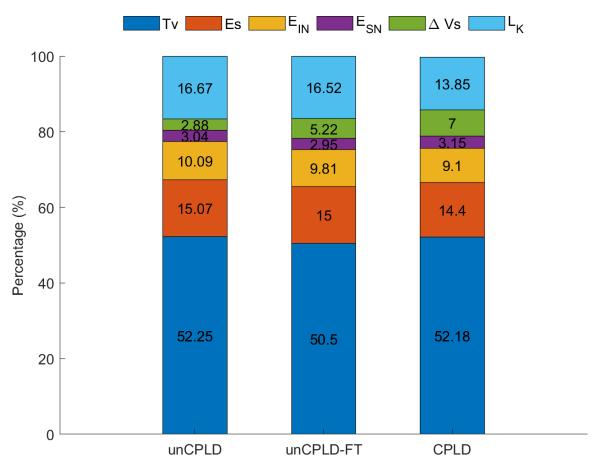


Figure 1011. Comparison of the relative ratios of different water budget components to precipitation during the whole simulation period produced by different model scenarios. Tv, transpiration; Es, surface evaporation; E_{IN} and E_{SN} , evaporation from intercepted canopy water and snow cover; Δ Vs, changes in soil water storage; L_{K} , deep leakage water.