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LETTER

Changes in soil water content and lateral flow exert large effects on soil thermal dynamics across Alaskan landscapes

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Abstract

Both lateral surface and subsurface water flow affect soil moisture dynamics, yet most land surface models only solve subsurface water movement vertically. Here, we use a 3D ecosystem model that considers both land surface and subsurface hydrologic processes to simulate soil moisture, which is then used to drive a 1-D vertical soil thermal model to simulate the soil moisture effects on soil thermal dynamics in central Alaska. Our coupled model improves soil temperature (ST) estimates by 43.5% in comparison with observational data. Soil moisture has little effect on ST during the wet season (−1.5%) and a substantial influence during the dry season (60%). Spatially, water lateral flow has significant impacts on both soil moisture and ST, causing model estimates for thawed areas in the transition season to increase by ∼10% in the study area. Our results highlight the importance of considering dynamical soil moisture, as well as lateral flow effects, on soil thermal dynamics in permafrost regions.

1. Introduction

Arctic land ecosystems play a significant role in affecting regional and global carbon cycling. About 1300 Pg of organic carbon is stored in Arctic soils, approximately one-third of global terrestrial organic carbon (Hugelius *et al* 2014, Mu *et al* 2015, Ofiti *et al* 2023). This substantial amount of organic carbon, stored mostly in permafrost regions, is vulnerable and highly sensitive to near-surface temperature change (Liu *et al* 2022), which could potentially cause positive feedback to the global climate system. Previous studies have shown that even with the most optimistic (minimum) warming rate, all permafrost in northwestern Alaska will completely thaw by ∼2200 (Batir *et al* 2017).

Among the various factors in modeling carbon dynamics of arctic land ecosystems, soil temperature (ST), and soil water content (SWC) are the two most crucial variables influencing biogeochemical processes (Oogathoo *et al* 2022). Previous studies have shown that the dynamics of STs and water can directly impact heat and moisture exchanges at the soil-air interface, which in turn affects water and carbon cycling (Decharme *et al* 2013). These dynamics also have considerable indirect impacts on the climate system by influencing other important processes, such as evapotranspiration within boreal forest ecosystems (Seneviratne *et al* 2010, Zittis *et al* 2014). ST and moisture have also been shown to be strong predictors of carbon fluxes from soils (Niinistö *et al* 2011). However, modeling the interactions within soil water and thermal dynamics, among many biogeochemical processes, remains a major challenge (García-García *et al* 2023).

Fan *et al* (2011) emphasized the importance of incorporating water flow into heat transport models to simulate future soil thermal and permafrost dynamics under a changing climate; other studies have also shown that subsurface lateral flow not only improves spatial characterization of soil moisture, but can also noticeably influence energy flux, partitioning transpiration, and ground evaporation (Kim and Mohanty 2016, Maxwell and Condon 2016). However, many land surface models (LSMs) still assume that lateral flow has minimal effect and therefore solves subsurface water movement only vertically (Zhuang *et al* 2003, Clark *et al* 2015, Liu and Zhuang 2023, Zhao and Zhuang 2024). These models are valid when the spatial resolution used is relatively coarse (Wood *et al* 2011, Schickhoff *et al* 2024). However, recent works suggest that lateral transport of subsurface water has significant influence on surface soil moisture and ground evaporation even at coarse resolutions (Ji *et al* 2017, Yang *et al* 2021). These studies also show that soil moisture and energy transport modeling demands using 1 km or higher resolution, especially during a dry season (Kannenberg *et al* 2024).

Some recent LSMs have the capability to simulate three-dimensional groundwater movement, but heat-transferring processes are typically excluded due to the complexity and prohibitive computing demands (Niu *et al* 2014, Liao *et al* 2019). Moreover, reconciling hydrological and thermal lower boundary conditions in these LSMs to simultaneously meet the requirements of simulating realistic ST profiles and modeling river discharges is still challenging. This difficulty arises because accurately simulating ST profiles requires soil to be sufficiently deep, while an adequately thin soil column is a prerequisite for simulating river discharges (Decharme *et al* 2013).

To overcome these difficulties in modeling soil hydrological and thermal dynamics, here we use a 1-D vertical terrestrial ecosystem model (TEM; Zhuang *et al* 2002) coupled with a process-based 3D hydrological and biogeochemical model (three-dimensional ECOsystem model; ECO3D; Liao *et al* 2019) to investigate the effects of the lateral flow of water and soil moisture on soil thermal dynamics in the Tanana Flats Basin, located in central Alaska. We first simulated soil water dynamics explicitly using the ECO3D model. We then used simulated soil moisture to drive the TEM model to improve the estimation of soil surface temperature and freeze-thaw dynamics across the landscape.

2. Method

2.1. Model description

The TEM is a highly aggregated large-scale process-based biogeochemistry model that uses spatially referenced information on climate, elevation, soils, and vegetation to simulate carbon and nitrogen dynamics, as well as water and heat processes within terrestrial ecosystems (Raich *et al* 1991, McGuire *et al* 1992, 2001, Melillo *et al* 1993, Zhuang *et al* 2001, 2002, 2003, 2004). To explicitly model the effects of soil thermal dynamics and terrestrial cryosphere processes on large-scale carbon dynamics within terrestrial ecosystems, a soil thermal module (STM) was developed and incorporated into TEM to represent heat fluxes within soil layers (Zhuang *et al* 2001, 2002, 2003). Tang and Zhuang (2011) further revised STM by incorporating a daily time-step snow model and including the moisture effects on soil heat capacity and thermal conductivity. In TEM, STs are estimated for each depth interval and time step for soil layers, but water and heat fluxes are only considered in the vertical dimension.

ECO3D is a three-dimensional TEM built upon an extant spatially distributed hydrological model, i.e. precipitation runoff modeling system (PRMS) and the TEM (Leavesley *et al* 1983, Markstrom *et al* 2015, Liao and Zhuang 2017a). Through the seamless coupling of water and carbon cycles, ECO3D can explicitly simulate lateral flow and its impact on carbon dynamics, thereby quantifying ecosystem production, consumption, and transportation of regional dissolved organic carbon (DOC) (Liao *et al* 2019).

Currently, ECO3D does not explicitly model soil thermal dynamics and TEM does not consider lateral movement of water. To investigate the combined impact of lateral water flow on SWC and thermal dynamics, we performed an offline coupling between ECO3D and TEM models. Specifically, in the previous version of TEM, SWC was assigned an initial value and calculated within the model simulation using the hydrology module (HM) that did not consider lateral water movement, which was then used to drive TEM soil thermal dynamics simulations. In this study, SWC simulated by ECO3D was used to drive TEM, representing the influence of both lateral and vertical water flow on soil moisture and soil thermal dynamics.

2.2. Study area and data

The Tanana Flats Basin is located near Fairbanks in central Alaska. The study basin is dominated by glacier and snowmelt-fed catchments with extreme relief from Mount Hayes in the eastern Alaska Range. Seasonal snowmelt is a major freshwater resource for most stream channels throughout the year. Surface elevation ranges from around 108 m on the Tanana Flat to about 3880 m at Mount Hayes in the study area (figure 1). In the northern part, as the Yukon River's largest tributary, the Tanana River, runs from east to west, from Big Delta to Nenana area. For decades until recently, the surface and groundwater as well as the soil thermal properties of this region have been continuously studied (Viereck *et al* 1993, Liao and Zhuang 2017a, Clayton *et al* 2021). The study area lies entirely within discontinuous permafrost zones under the current climate where approximately 60% of the soil is underlain by permafrost (Liao and Zhuang 2017b). To date, much attention

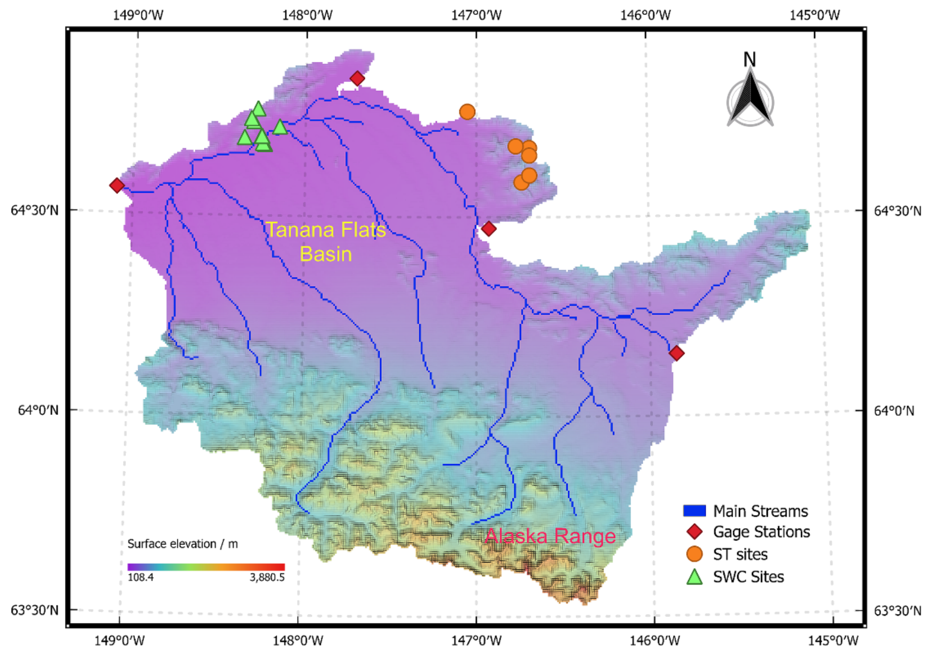

Figure 1. Topography of the study basin: Blue lines are streams; green triangles represent the eight soil water content data sites; orange dots represent the six soil temperature data sites; red squares represent four USGS gage stations (table S2).

has been paid to studying ecosystem dynamics, permafrost degradation, decrease in glacier volume, and snowmelt pattern changes in this region (Jorgenson *et al* 2001, 2020, Hill *et al* 2015, Liao and Zhuang 2017b).

For both our 3D and 1-D simulations, the horizontal spatial resolution is set to 500 m, and the study period is 2002–2022. Therefore, *in situ* climate data from global historical climatology network (GHCN) and global summary of the day (GSOD) through NOAA's national centers for environmental information (NCEI) (Menne *et al* 2012) was interpolated to the spatial domain using the Kriging method and the ANUSPLIN package (Xu and Hutchinson 2013) to provide spatially explicit data. After processing, daily (for ECO3D) and monthly (for TEM) climate data were produced at 500 m resolution for model simulation. 1 km × 1 km resolution daily cloud fraction data were obtained from the moderate resolution imaging spectroradiometer (MODIS) Cloud Mask product (MOD 35) (Ackerman and Frey 2015) and then resampled to 500 m monthly resolution only as input for TEM simulation. Time invariant polygon-based soil type data, 60 m resolution digital elevation model (DEM) data, and 30 m resolution land use and land cover change (LULCC) data were derived from the Natural Resources Conservation Service soil survey geographic database (SSURGO data sets) (Soil Survey Staff 2023), the USGS National Elevation Dataset (NED) (Gesch *et al* 2002), and the national land cover database (NLCD) (Fry *et al* 2011) separately, and then processed to fit both ECO3D and TEM simulation. Data for four gage station stream discharges from the U.S. Geological Survey Gage (USGS) were used as ECO3D model input to represent the studied basin received streamflow from upstream (U.S. Geological Survey 2016). Daily MODIS Leaf Area Index/ FPAR products (MOD15A2H) were also used to consider the temporal variation impacts of canopy density (Myneni *et al* 2015). The description of the data used is summarized in table S1.

2.3. Soil moisture effects on soil thermal properties

In the TEM-STM model (Zhuang *et al* 2002, Tang and Zhuang 2011), soil heat conductivity was computed based on the Kersten number (K_e), which is estimated based on the degree of soil saturation θ_{sat}. The Kersten number for unfrozen soils ($K_{e,\mathrm{uf}}$) and soil saturation are calculated as (Balland and Arp 2005):

$$K_{e,\mathrm{uf}} = {\theta_{\mathrm{sat}}}^{0.5(1+V_{\mathrm{om},s}-\alpha V_{\mathrm{sand},s}-V_{\mathrm{cf},s})} \times \left[\left(\frac{1}{1+\mathrm{e}^{-\beta\theta_{\mathrm{sat}}}}\right)^3 - \left(\frac{1-\theta_{\mathrm{sat}}}{2}\right)^3\right]^{1-V_{\mathrm{om},s}} \quad (1)$$

$$\theta_{\mathrm{sat}} = \frac{V_{\mathrm{t}}}{V_{\mathrm{pores}}} \quad (2)$$

where α and β are the adjustable parameters. $V_{\mathrm{om},s}$ $V_{\mathrm{sand},s}$, $V_{\mathrm{cf},s}$ are the volumetric fractions of organic matter, sand, and coarse fragments within the solid soils, respectively. V_{t} is total volumetric water content (VWC) and V_{pores} is soil porosity.

When soil is frozen or partially frozen, Kersten number ($K_{e,\mathrm{f}}$) is calculated as:

$$K_{e,\mathrm{f}} = {\theta_{\mathrm{sat}}}^{1+V_{\mathrm{om},s}}. \quad (3)$$

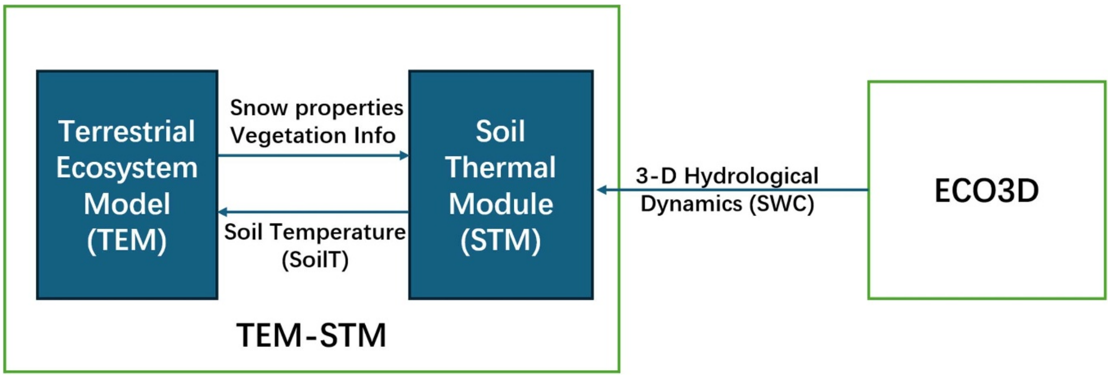

Figure 2. The structure of ECO3D-TEM-STM coupling. ECO3D-output SWC is passed to TEM-STM.

For both frozen and unfrozen soils, the volumetric heat capacity is computed as:

$$C_{\mathrm{vol}} = \sum_i V_i C_{\mathrm{vol},i} \tag{4}$$

where V_i is volumetric fraction of different soil matter, air, liquid water (V_{water}) and ice (V_{ice}). From which V_{water} and V_{ice} for each layer is determined as a function of ST and total VWC V_{t} incorporated from Decker and Zeng (2006):

$$\frac{V_{\mathrm{ice}}}{V_{\mathrm{t}}} = \frac{1 - \exp\left[\alpha \times \left(\frac{V_{\mathrm{t}}}{V_{\mathrm{s}}}\right)^{\beta} \times (T - T_{\mathrm{frz}})\right]}{\exp\left(1 - \frac{V_{\mathrm{t}}}{V_{\mathrm{s}}}\right)} \tag{5}$$

where V_{s} is the saturated volumetric moisture content, α and β are empirical parameters, chosen 3 and 2 respectively, T_{frz} is the reference temperature for freezing.

Although the effect of soil moisture on soil heat capacity and thermal conductivity was considered, the total VWC was prescribed for each soil layer during the model set-up and then calculated without considering the lateral water flow in TEM-STM. In this study, we substituted V_{t} with ECO3D-simulated dynamic total SWC (figure 2). Therefore, by feeding the 3D modeled total SWC into equations (1)–(5), the coupled model explicitly simulates the impact of lateral water flow on SWC and its influence on soil heat capacity and soil heat conductivity, thereby soil thermal dynamics.

2.4. Experiment design and observation data

We first simulated the 1 m average SWC for the study area using the ECO3D model. We then evaluated the results by comparing them with site-level observations to analyze temporal patterns. Hourly soil moisture measurements (VWC) from the study area and period (figure 1) at various depths (5 cm, 20 cm, 50 cm) in the Bonanza Creek experimental forest near Fairbanks, Alaska (Bonanza Creek LTER program, BNZ LTER; Chapin *et al* 2022), were collected from eight upland and floodplain sites and averaged to the daily time step to match the model output resolution. Site information is summarized in table S2.

Table 1. Simulation design.

Model used	Input data	Outputs for analysis
ECO3D	Climate, LAI/FPAR, stream discharge, LULCC, soil type	Soil water content (SWC)
Original TEM-STM	Climate, cloud fraction, LULCC, soil type	Soil temperature at top 5 cm soil depth (ST)
Revised TEM-STM	Climate, cloud fraction, LULCC, soil type, SWC from ECO3D output	Soil temperature at top 5 cm soil depth (ST)

After validating the ECO3D simulated SWC, we then applied it to drive our TEM-STM model. To ensure data consistency, all the input data used to drive TEM were either the same data used to drive ECO3D (climate data), or data derived directly from ECO3D output (SWC), except for cloud fraction data. For site-level comparisons, daily soil surface temperature at a depth of 3 cm from six different sites in the study area (figure 1) during the study period was collected from NASA Arctic-boreal vulnerability experiment (ABoVE) project (table S2). TEM outputs surface ST at a monthly step, site measurements were also aggregated to the same time resolution. Three simulations are conducted (table 1).

3. Results

3.1. SWC

We first evaluated shallow layer SWC simulated with ECO3D at the site level (figure 3). TEM-calculated soil liquid water content (V_{w}) using equation (5) is also evaluated during the soil frozen period. In general, the temporal pattern of the monthly averaged SWC aligned well with the measured VWC at the

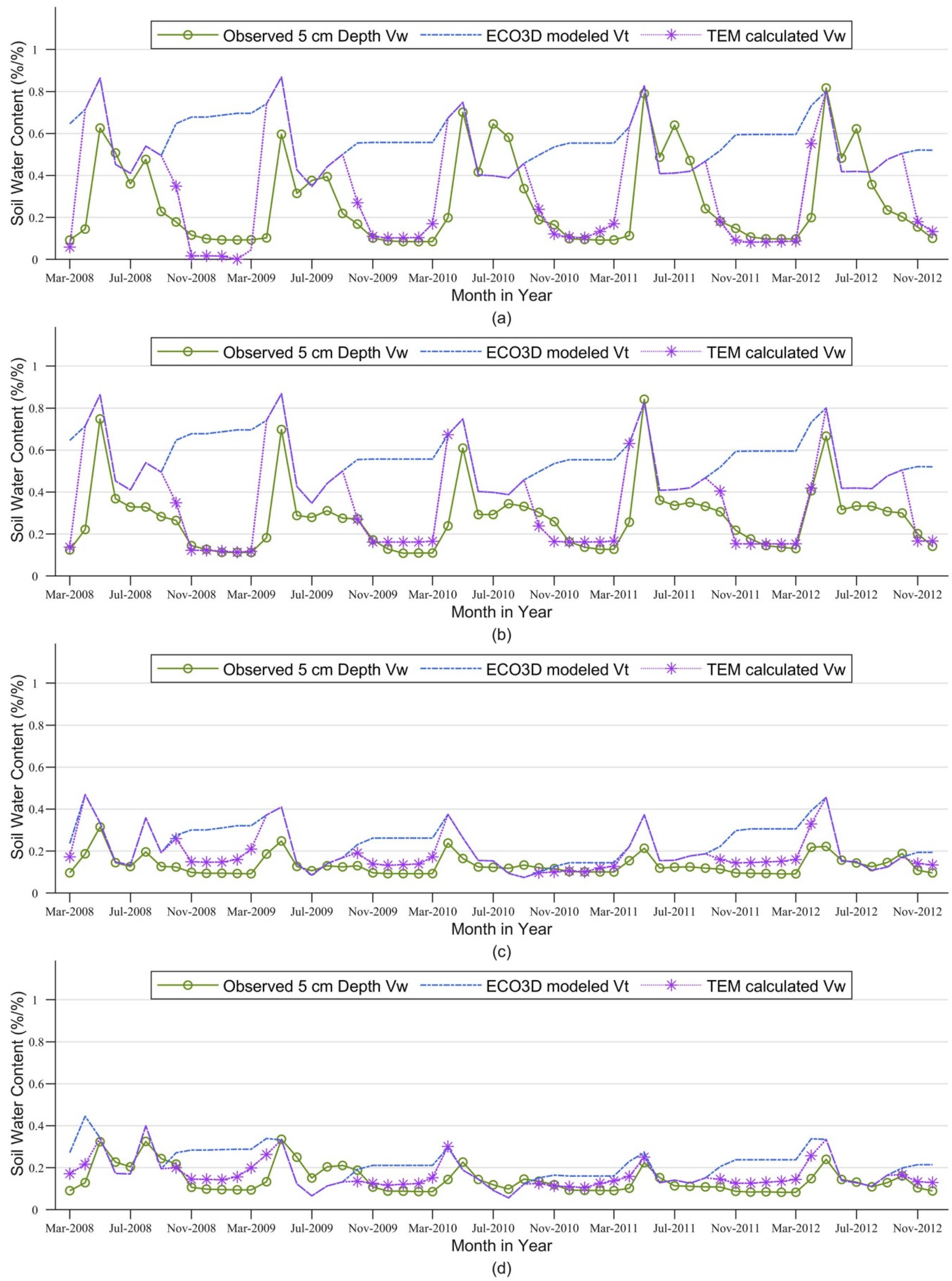

Figure 3. Comparison between ECO3D output total soil water content (SWC/V_t), TEM calculated soil liquid water content (V_w) during frozen season and measured 5 cm depth volumetric water content (VWC/V_w) at site FP1A (a), FP2A (b), UP1A (c), and UP2A (d) (table S2).

5 cm depth. When soil is unfrozen, ECO3D estimated monthly SWC value is close to measurements with a similar trend from April to September. Even in the daily comparison (figure S1), ECO3D captured the SWC trend during the unfrozen season, especially for the sudden rise in late April and the sharp fall in mid-May, as well as subsequent fluctuations in shallow soil VWC (5 cm).

However, during the frozen season (late September to early April), the ECO3D-simulated SWC remained stable after a slight increase typically starting from early November, while the observed soil moisture with an opposite pattern. It displayed a gradual decline from around September, followed by a sudden drop, where the timing varies based on the depth of the soil (figures 3 and S1). During

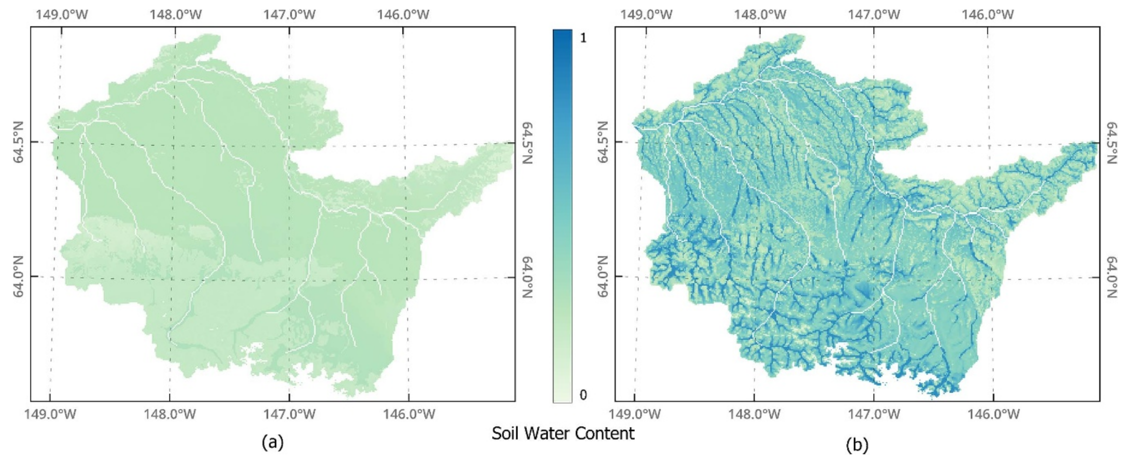

Figure 4. Total volumetric soil water content in May 2013 modeled by TEM-STM (a) and ECO3D (b), with an average value of 0.22 and 0.55, respectively.

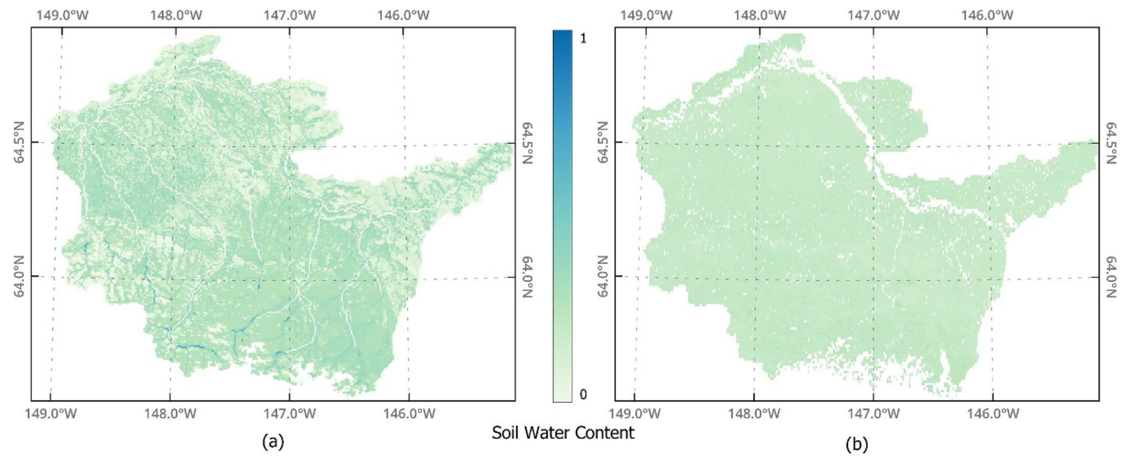

Figure 5. Comparison surface soil moisture in August 2012, (a) is ECO3D model simulation, (b) is from GSSM 1 km dataset (Han *et al* 2023) with an average value of 0.21 and 0.19, respectively.

this period, TEM calculated V_w matches both the value and trend with the observed shallow V_w, with the only exception for several transitional months (March/April and September /October) where the monthly ST is above the freezing point.

3.2. Spatial pattern of lateral flow and its impacts

By explicitly simulating the lateral flow, ECO3D is able to show the impact of lateral flow on SWC. The averaged spatial SWC for May 2013 indicates the influence of lateral flow (figure 4(b)). In the southwestern high mountainous region where Mount Hayes is located, the hillslope lateral flow, has a more pronounced effect than in the central lowland and the northern Tanana Flats. In contrast, the 1-D model simulation not only underestimates SWC (0.22 vs 0.55), but also shows no lateral flow pattern (figure 4(a)). We also compared our results with global surface soil moisture (GSSM1 km) data, a high-resolution product generated from a physics-informed machine learning method using international soil moisture network (ISMN), remote sensing, and meteorological data to provide surface soil moisture (0–5 cm) at 1 km spatial and daily temporal resolution over the period 2000–2020 (Han *et al* 2023). We averaged the surface soil moisture results for August 2012 from both model products (figure 5). Although the two datasets differ in spatial resolution (500 m vs 1000 m), their magnitudes are similar (0.21 vs 0.19). In addition, the ECO3D model shows more spatial details due to lateral flow impacts, whereas GSSM 1 km data exhibit less variations, probably due to the sparse coverage of the ISMN network in this region.

3.3. Temporal variations of ST

Simulated ST from the revised model differed little from the original model simulation, both being close to field measurements from June to October (figure 6). Original model simulation was slightly closer to observations by 1.5% with root mean square error (RMSE). However, from October to May, the

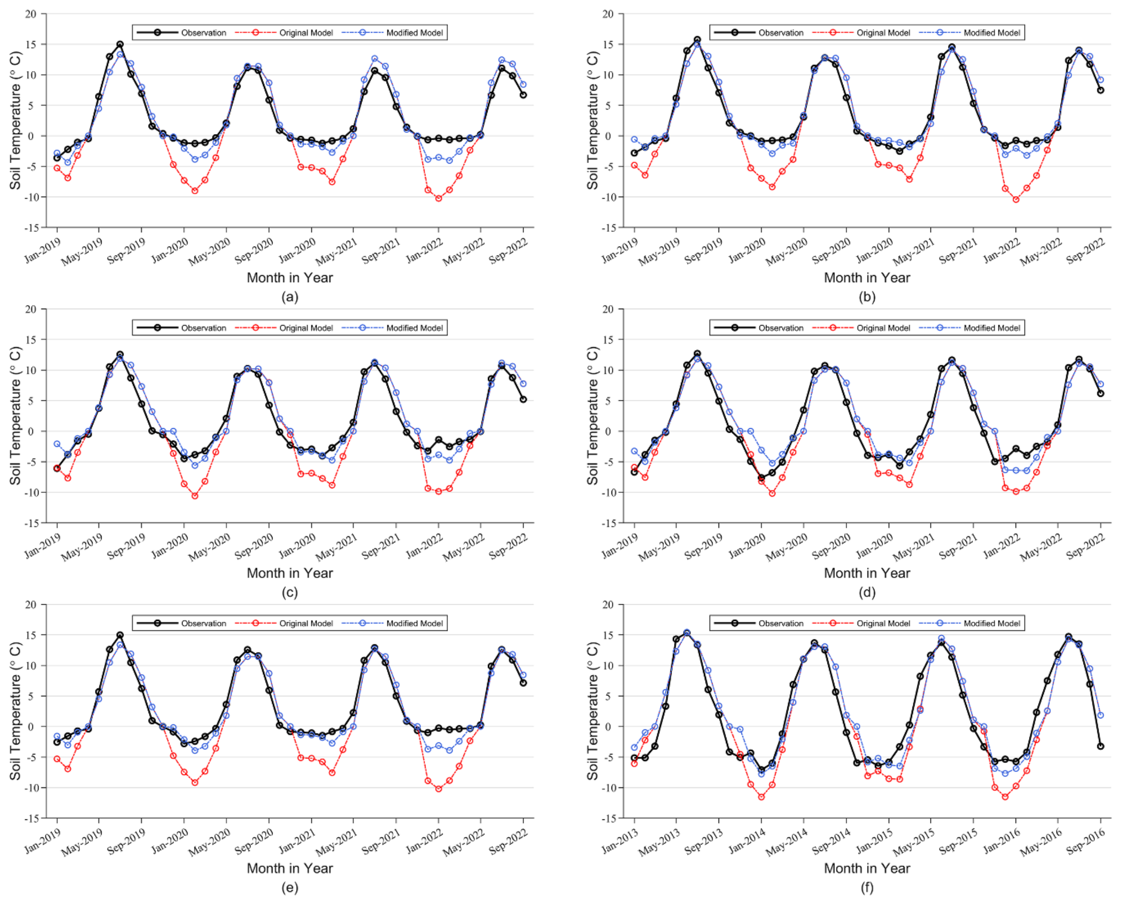

Figure 6. Comparison between both original and revised TEM-STM simulations and observational temperature at 5 cm soil depth at sites YTA-UWNB2 (a), YTA-UWNB3 (b), YTA-UWNU1 (c), YTA-UWNU3 (d), YTA-UWNB1 (e), and HL-BM (f).

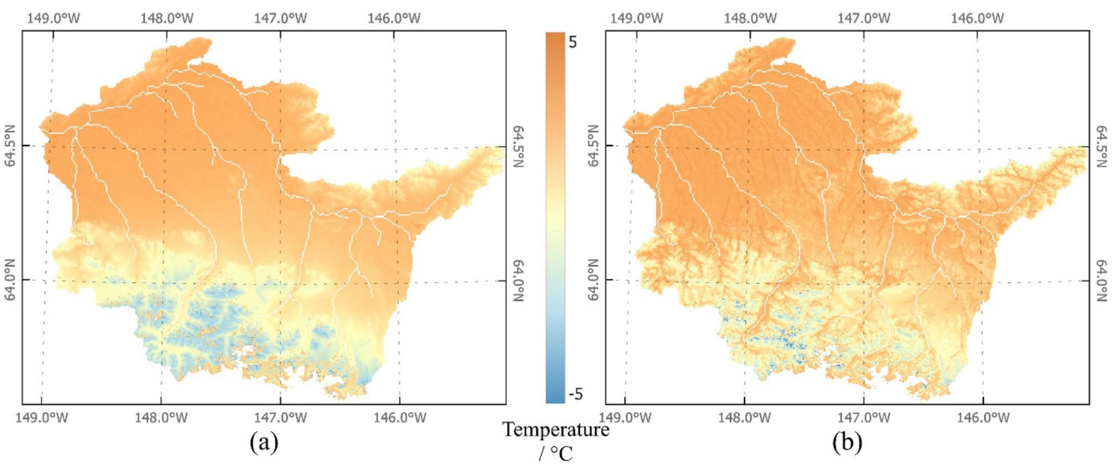

Figure 7. Mean monthly soil temperature for May 2013: (a) is original model simulation, (b) is the revised model simulation.

revised model simulation is significantly closer to the observations. In addition, the revised model markedly matched the trend of the observations, especially from December to February. During this period, the revised model improved the simulation accuracy by 57.9%, based on a six-site average RMSE. Overall, by incorporating lateral flow effects on SWC, our modified model improved the ST simulation by 43.5%.

Driven by 3D dynamic SWC, the revised TEM-STM represents the impact of lateral flow on ST (figure 7). In May 2013, the spatial SWC (figure 4) shows a different pattern from ST. In the southwestern high mountainous region, ST is relatively lower due to low air temperature at higher elevations, but around the main channels (figure 1), ST remains significantly higher than the original model simulations (figure 7(a)). In the central basin and the northern

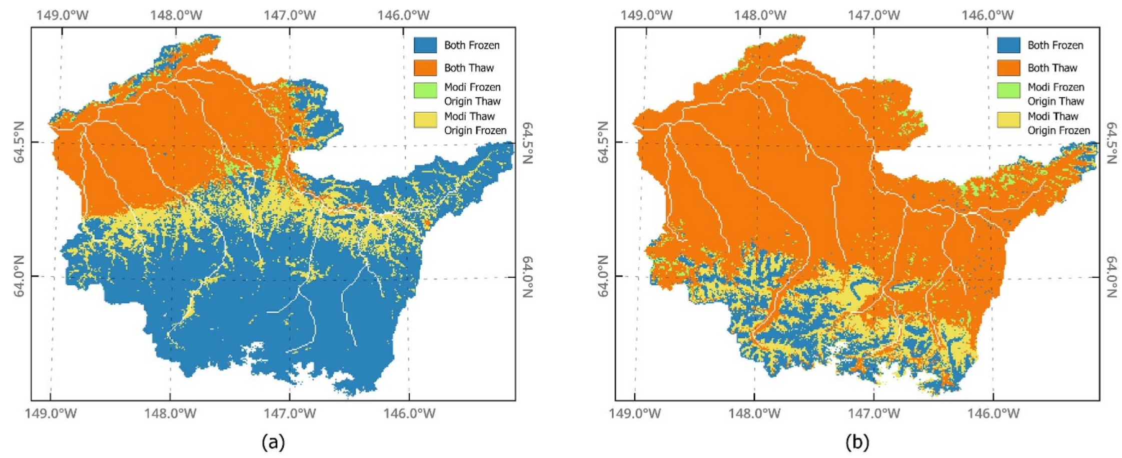

Figure 8. Freeze-thaw status in two transitional months of April (a) and October (b) in 2012 estimated with the original (Origin) and the modified TEM-STM (Modi).

Tanana Flats, ST shares a similar spatial variation to SWC.

Changes in surface STs could have considerable influence on ground freeze/thaw status (F/T), particularly for soils in the transitional seasons. To obtain the ground F/T status, an average surface ST of −0.9 °C was used as a freezing threshold to separate frozen soil from thawed status (Rivkina *et al* 2000, Kozlowski 2004, 2009). Two months during transitional seasons were calculated including April 2012 (figure 8(a)) and October 2012 (figure 8(b)). Two versions of TEM-STM results largely agree in most areas. However, some discrepancies appear in transitional zones (figure 8). The revised model estimated more unfrozen/thawed areas (9%–12%) for April and October, which was caused by soil moisture effects on ST.

4. Discussion

4.1. Temporal variation of SWC

The comparison between modeled and measured SWC shows that ECO3D performed well in simulating soil water dynamics during the unfrozen season (May to September). The model captured the fluctuating trend, especially in shallow soil layers (5 cm and 20 cm; figures 3 and S1), since deep SWC changes more gradually and with a time lag. However, during the completely frozen season (November to March), the model performs poorly in capturing soil moisture/liquid water content. The reason is that ECO3D lacks soil thermal dynamics (Liao *et al* 2019). Consequently, the SWC in ECO3D does not separate ice/water for the whole vertical soil profile, meaning that its SWC output reflects total soil water (including ice) rather than volumetric liquid water content. Therefore, during the frozen season, the high but steady SWC value not only indicates weak lateral flow due to the frozen soil surface, but also states that some part of the soil is completely frozen. Nevertheless, observed deep soil water still shows some active movement during the frozen season, even when shallow soil is completely frozen (figure S1). Previous studies also suggested that despite soil surface temperatures falling below 0 °C causing soil water to freeze to 10 cm depth, deeper soil layers at 30–90 cm depth often retain predominantly unfrozen soil water (Brandt *et al* 2020). Sutinen *et al* (2008) found that during mild climatic events in early winter, snowmelt releasing water was observed to infiltrate through partially frozen soil, thus increasing the deeper unfrozen SWC. Oogathoo *et al* (2022) also noted a relatively less consistent and less pronounced peak for SWC during the autumn and contributed to the decrease in evapotranspiration coinciding with the end of the growing season. These studies could explain the sudden rise in our simulated SWC around November and the subsequent stable high values.

4.2. Lateral flow impacts on spatial and temporal ST

ECO3D does not consider phase change during the frozen season while the STM in TEM could accurately model the vertical dynamics of soil water/ice (Zhuang *et al* 2003, Tang and Zhuang 2011). Soil water dynamics and lateral flow seem to have less impact on soil thermal properties during the warm season (June to October), but considerably influence these properties in the cold season (November to May) (figures 4, 6 and 7). Both the original and revised TEM-STM models captured the real soil thermal regime during the warm season due to two reasons. First, ST has a low sensitivity to SWC during this period, as reflected in the model algorithm (equation (1)), where θ_{sat} has little influence on K_e. The second reason is, during the warm season, ECO3D modeled SWC closely matches the TEM-prescribed values, causing the K_e values closer as well, thus minimizing their differences in modeled ST. However, in the cold season, the total water content increases ST, causing it to be closer to measured data, while the original model without dynamic SWC fails to match both observed ST and its trends. This is because θ_{sat} plays a more important role in influencing K_e (equation (3) in the partially or completely frozen soils. Although soil water may partially freeze during this period, water and ice collectively influence soil thermal conductivity as a single parameter (θ_{sat}). ECO3D represents this correctly, under the validation using equation (5) (figure 3), whereas the prescribed value in TEM greatly underestimates it. A recent study shows that soils may be frozen in the tundra, ST observations at the boreal forest site, however, rarely drop below 0 °C (Oogathoo *et al* 2022). This is consistent with our model simulations for tundra sites (figures 6(d) and (f)) and boreal forest or woodlands sites (figures 6(a), (b) and (e)). At a regional scale, SWC and the revised model simulation of ST have a similar spatial pattern (figures 4 and 7(b)), highlighting the effect of soil water on soil thermal properties.

4.3. Uncertainty analysis

Our revised modeled ST compared well with observations, emphasizing the importance of lateral flow effects on soil thermal dynamics. Yet, some issues need to be addressed in future studies. First, our revised model is a one-way offline coupling, which only considers the impact of dynamic soil water and lateral flow on soil thermal properties, while ignoring the reverse influence due to the lack of a soil thermal model in ECO3D. This results in unrealistic soil moisture output that contains ice during the frozen season. Recent studies have also suggested that the soil moisture and ST feedback shall be represented within LSMs (García-García *et al* 2023).

Second, due to lacking high-resolution observation data, the climate input data used in our simulations are based on site-level interpolation. Although the interpolation methods we used have taken elevation into account and have been widely used (Xu and Hutchinson 2013), they may still introduce certain uncertainties. Moreover, our revised model simulations still show some discrepancies during the cold season compared to observations, suggesting other processes and factors might also affect ST simulations, for instance, snow or vegetation dynamics (Xu and Zhuang 2023).

Our future research is to establish a two-way coupling between ECO3D and TEM-STM to simultaneously consider the soil thermal and hydrological dynamics and their interactions. Additional processes of interactions between snow, permafrost, and vegetation dynamics shall also be considered to improve ST and freeze-thaw estimation in boreal regions.

5. Conclusions

This study uses an offline coupling between a 3D process-based hydrological and biogeochemical model ECO3D and a 1-D vertical TEM to examine the effects of both lateral and vertical water flow on soil moisture and soil thermal dynamics. During the study period, our coupled model improved the accuracy of the simulated ST by 43.5% in comparison with observed data. Our simulations indicate that soil moisture has minimal effects on ST during the warm season (−1.5%) but has a substantial influence during the cold season. When considering only the cold season, the coupled model improved the soil surface temperature simulation accuracy by 60%. Spatially, the lateral flow shows significant impacts on both soil moisture and ST. These results emphasize the importance of considering dynamic soil moisture and lateral flow effects on ST in TEM.

Data availability statement

The data used to reproduce figures, codes, model and samples of running directory can be accessed via Purdue University Research Repository: https://purr.purdue.edu/publications/4743/1. The revised TEM-STM model source code is available at https://github.com/AlexLiuxy/Revised-TEM-STM-ECO3D. The ECO3D model can be accessed at: https://github.com/changliao1025/eco3d.

The data that support the findings of this study are openly available at the following URL/DOI: doi:10.4231/XQ71-GN27 (Zhuang and Liu 2024).

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Conflict of interest

The authors declare that they have no conflict of interest.

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