Inferring Permafrost Active Layer Thermal Properties From Numerical Model Optimization

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Abstract  Permafrost has become increasingly unstable as a result of surface warming; therefore it is crucial to improve our understanding of permafrost spatiotemporal dynamics to assess the impact of active layer thickening on future hydrogeological processes. However, direct determinations of permafrost active-layer thermal properties are few, resulting in large uncertainty in forecasts of active layer thickness. To assess how to reduce the uncertainty without expanding monitoring efforts, a total of 1,728 numerical 1D models were compared using three error measures against observed active layer temperature data from the Qinghai-Tibetan Plateau. Resulting optimized parameter values varied depending on the error measure used, but agree with reported ones: bulk volumetric heat capacity is 1.82–1.94 $\times 10^6$ J/m$^3$ K, bulk thermal conductivity 1.0–1.2 W/m K and porosity 0.25–0.45. The active layer thickening rate varied significantly for the three error measures, as demonstrated by a ~15 years thawing time-lag between the error measures over a 100 years modeling period.

Plain Language Summary  In Arctic permafrost regions, the thickness of the active layer, the top soil layer subjected to seasonal freezing and thawing, is increasing as a result of increasing air temperatures. Consequently, increasing amounts of the greenhouse gases of carbon dioxide and methane could be released into the atmosphere and the regional hydrology and vegetation will change. Models are used to study the development of the active layer, which are based upon parameters that represent properties found in the field. In this study, we compare observed temperature data from the active layer to results from 1,728 unique models with varying parameters using three error measures. We determined which parameters can best mimic the observations, without the need to collect samples in the field. This method can help improve the accuracy of models, enabling researchers to better understand the processes involved in increasing active layer thickness and to make more accurate forecasts of future active-layer behavior.

1. Introduction

Permafrost has become thermally unstable over the past few decades as a result of rising air temperatures (Biskaborn et al., 2019; Romanovsky et al., 2002; Vonk et al., 2015). The degradation of permafrost commences with an increasing thickness of the active layer toward the end of summer (Bense et al., 2012; Koven et al., 2015; Schuur et al., 2008; Walvoord & Kurylyk, 2016). A deepening of the active layer signals the onset of permafrost degradation, which has been widely observed using long-term observations of shallow (e.g., < 10 m) temperature profiles (Abramov et al., 2019; Åkerman & Johansson, 2008; Luo et al., 2016; Wu et al., 2015). Increasing active layer thickness has a direct impact on many environmental processes including hydrology (Bense et al., 2009; Frey & McClelland, 2009; Kurylyk et al., 2013), the water quality of aquatic ecosystems (Toohey et al., 2016) and results in fundamental landscape and vegetation change through thermokarst processes (Bouchard et al., 2014; Prowse et al., 2006; van der Kolk et al., 2016). Longer-term impacts at large spatial scales include the development of deeper groundwater flow pathways which can induce more vigorous groundwater solute transport (Bense et al., 2012; Frampton et al., 2013; Walvoord & Striegl, 2007; Walvoord et al., 2012), thereby changing regional hydrogeological systems.

The timescale on which environmental processes are affected by permafrost thaw is uncertain (Andresen et al., 2020). One of the most important rivers of China, the Yellow River, originates on the Qinghai-Tibet Plateau (QTP) (Cheng & Jin, 2013). Groundwater discharge originating from the thawing permafrost could undergo significant changes as the active layer increases in thickness (Song et al., 2020; A. Sun et al., 2020;
T. Wang et al., 2018). The local population relies on a stable discharge because water is used for irrigation and electricity production (Ding et al., 2017; Penghao et al., 2019). The timescale on which river discharge may change is therefore crucial in planning adaptation measures. Furthermore, active layer thickening is expected to lead to the mobilization of organic carbon and other constituents such as Hg (O’Donnell et al., 2012; Schuster et al., 2018; Schuur et al., 2009; Turetsky et al., 2020), which can emerge from the thawing permafrost (Vonk et al., 2019; Zimov et al., 2006). Groundwater chemistry changes in turn affect microbial activity, which is responsible for organic matter decomposition and release of CO₂ and CH₄ into the atmosphere (Keller et al., 2010; Mondav et al., 2017; Schuur et al., 2008; Walz et al., 2017). The primary release mechanism of CO₂ and CH₄ from the active layer has been surface erosion and direct oxidation and release into the atmosphere (Dutta et al., 2006), yet with a deepening active layer, migration through groundwater will gain a more prominent role (Walvoord & Striegel, 2007). With over 818 Gt of organic carbon stored in the top 3 m of the northern hemisphere active layer, a vast amount of CO₂ and CH₄ could potentially be released into the atmosphere (Dutta et al., 2006; Schaefer et al., 2011; Tarnocai et al., 2009; T. Wang et al., 2020). Additional release of CO₂ and CH₄ into the environment will affect current global warming predictions and may accelerate subsequent processes such as sea level rise. It is of vital importance to understand the timescale on which the active layer thickening occurs and to better understand uncertainties in predictions of permafrost active layer thickness in the coming century.

Heat transfer models are used to simulate active layer freeze-thaw dynamics, and require thermal properties, including thermal conductivity λ and heat capacity C, to quantify heat transfer processes. In order to model active layer development over large areas, spatial data on subsurface thermal properties are required. Yet such data are scarce, requiring field sampling and laboratory analysis. Therefore, the subsurface thermal properties are often estimated using empirical relations with surface indicators such as soil texture, soil type, and vegetation (Luo et al., 2014; Zhao et al., 2017; S. Zhao et al., 2017). However, uncertainties are introduced when translating surface data of large areas into subsurface thermal properties because the relation between surface phenomena and subsurface thermal properties is not evident (Kitover et al., 2016; S. Zhao et al., 2017). Therefore, more accurate data on active layer thermal properties is required. Active layer properties λ and C can be accurately measured from field samples (D. Zhao et al., 2016). The thermal diffusivity, which is the ratio between λ and C can be determined using field temperature observations (Arias-Penas et al., 2015; Carson, 1963; Gao et al., 2017; Hinkel, 1997; Q. Liu et al., 2019). For modeling purposes, individual λ and C values are often required, which depend on specific subsurface properties; for example, parent material, organic matter content, air, and (un)frozen soil moisture content (Midtømme & Roaldset, 1998; Mustamo et al., 2019). Reported bulk thermal conductivity (λ) of the subsurface ranges from 0.05 to 2.2 (W/m K) for active layers in Alaska, Siberia and the QTP (Brouchkov et al., 2005; Chen et al., 2020; Romanovsky & Osterkamp, 2000) and specific heat capacity (C) ranges between 580 and 690 (J/kg K) (Chen et al., 2020; L. Liu et al., 2018). Such data are not available for large parts of degrading permafrost areas. As a consequence, active layer thermal property variability—which is mostly unknown due to the active layer’s composition and dynamic boundary condition behavior—leads to a high degree of uncertainty when modeling active layer thawing depth and timing of thawing events (Schaefer et al., 2011).

In this study we demonstrate that permafrost temperature observations in combination with a numerical 1D heat transfer model can be used to evaluate thermal properties λ and C. We used the transient heat transfer equation (Grenier et al., 2018; Kurylyk et al., 2014) to model a batch of active-layer temperature time series. The 1D model is kept as generic as possible and excludes stratification to demonstrate that effective thermal property values can be obtained with very limited site-specific stratigraphic data. Thereafter, we used three types of error measurements: Root Mean Squared Error (RMSE), Kling–Gupta Efficiency (KGE) and Russell’s error to find the best fitting models with associated thermal properties to match the temperature field observations. The resulting three optimal parameter combinations are subsequently used to model a 100 years future scenario, investigating the effect of the contrasting optimum parameter values on long-term predictions of active layer depth, thawing rate, and the degradation of deeper permafrost.

The selection of a particular error measure is often determined by the error measure that is, commonly used by the researcher in their field. However, careful consideration should be made regarding the type of data that is being used and the modeling objective (Jakeman et al., 2006). The choice for one specific error measure could create systematic bias, translating into an error that is omitted in the parameter sensitivity.
analysis. The RMSE and KGE error measures are common when evaluating models with observational data, where RMSE evaluates the residuals—the difference between observation and data—and KGE also takes the bias into account (Bennett et al., 2013). Since we are investigating the timescale of thawing events, we want to pay particular attention to the difference in timing (phase errors) as well. Therefore we also use the Russell’s error, which combines a phase and magnitude error to evaluate time series that are subjected to a phase shift (Russell, 1997).

2. Active Layer Thermal Dynamics Observed on the Qinghai-Tibet Plateau

The QTP is an area subjected to ongoing permafrost research, where a relatively large quantity of temperature observations are being collected (Hu et al., 2019; Wu et al., 2010; Zou et al., 2017). We used field data from one site on the QTP (34°15.3’N and 97°51.2’E) as reported in Luo, Jin, Wu et al. (2018) and Luo, Jin, He, et al. (2018). These consist of shallow temperature observations (at depths of 5 cm, 20 cm, down to 200 cm at a 20 cm interval) collected between November 2010 and December 2016, using a thermistor chain. The QTP is an elevated permafrost plateau region situated in China at an altitude between 4,600 and 4,750 m above sea level. Mean long-term annual air temperature is −4.5°C and annual precipitation is about 460 mm, mainly occurring from May to September (Luo, Jin, He, et al., 2018). The mean permafrost temperatures on the QTP reach approximately −2.0°C (Cheng & Wu, 2007; Wu et al., 2010). Observations over the period 1980–2000 indicate that the mean permafrost temperatures increased by 0.2°C during the observed period (Cheng & Wu, 2007; Jin et al., 2009; G. Wang et al., 2007). The permafrost in this area has been degrading and decreasing in extent over the past decades, and continues to do so as a result of sensitivity to temperature increase (Cheng & Jin, 2013; Luo et al., 2016; Ran et al., 2021; Wu & Zhang, 2008; Wu et al., 2010). Regionally, the QTP contains a mixture of continuous, discontinuous, and sporadic permafrost (Jin et al., 2009) and there is a strong variability in soil texture, soil moisture, and peat occurrence (Li et al., 2016). The soil at the measurement location is composed of a poorly drained organic layer of 0.2–0.3 m with high moisture content. Beneath the organic layer, a peat layer extends 0.5 m which is underlain by silty sands and coarse gravel (Luo, Jin, He, et al., 2018; Luo, Jin, Wu, et al., 2018).

The temperature data set includes continuous daily temperature observations. The data illustrate typical behavior for freeze-thaw cycles where different stages can be distinguished (Figure 1a), namely, (a) the zero-curtain period during which pore water freezes, controlled by the release of latent heat (Puukonen, 1998; Romanovsky & Osterkamp, 2000), (b) Sub-zero temperatures, with stable thermal properties, (c) ice phase transition back to the water, dynamic thermal properties, and (d) above 0°C ground temperatures, fast response to air temperature fluctuations. Figure 1b shows the maximum active layer depth where the temperature exceeds 0°C interpolated from the observed data.

3. Methods

3.1. Numerical Modeling

In this study we implemented the conduction heat transfer equations (Bense et al., 2009; Frampton et al., 2011; Grenier et al., 2013; McKenzie et al., 2007; Nagare et al., 2015; Sjöberg et al., 2016), using the FlexPDE software package (PDE Solutions, 2020) as our numerical modeling environment. A 1D model with solely vertical conductive heat transport was constructed. Lateral heat flow will be very limited in the semi-frozen saturated conditions and the lack of topography at the site on the QTP that we consider here. The permafrost model incorporates the 1D equation for conductive heat transfer written as:

\[ \frac{\partial^{\lambda_{f}}}{\partial t} \left( \lambda_{f} \frac{\partial T}{\partial z} \right) = C_{v} \frac{\partial T}{\partial t} + \phi L \frac{\partial S_{w}}{\partial t} \]  

(1)

We assumed fully water-saturated subsurface conditions. The transient freeze-thaw heat flow processes include consideration of pore water phase change and the required latent heat of fusion, which is governed by the water saturation curve described here by an exponential function. Volumetric heat capacity \( C \), thermal conductivity \( \lambda \) and porosity \( \phi \) are soil-specific properties and water versus ice saturation equations are a function of soil properties and temperature. Porosity \( \phi \) controls the pore water fraction, and thereby \( \lambda_{f} \).
Parameter values are listed in Table 1. The combination of \( \phi \) (6 values), thermal conductivity of the solids \( \lambda_s \) (16 values) and volumetric heat capacity of the solids \( C_v \) (18 values) were varied, resulting in a total of 1,728 simulations. Parameter value ranges represent a parameter space covering minimum to maximum values common for permafrost areas as presented in the introduction.

The 1D model represents a vertical domain of 30 m, in which the top 2 m is of particular interest as this is where we have validation data available. The top boundary \( (T_{top}) \) was forced by a data set composed of the observed temperature at 5 cm depth. We smoothed this forcing data set to mitigate large jumps in temperature forcing, which avoids numerical instability at the boundary. By utilizing the observations at a depth of 5 cm, instead of air temperature, surface-atmosphere boundary effects and the effects of potential snow or vegetation insulation did not have to be taken into account in our model description, which would have been difficult to constrain (Fisher et al., 2016; L. Liu et al., 2018). The bottom boundary \( (T_{bottom}) \) had a fixed temperature of −1.12 °C, which was found by linearly extrapolating the depth profiles at all given timesteps to attain a realistic average temperature gradient of 0.02°C/m to a depth of 30 m. The fixed value for \( T_{bottom} \) is realistic since little change in temperature at that depth over the model period of 6 years is expected. See the supplementary material for the conceptual model, applied boundary conditions, and observed temperatures. There is an organic-rich layer in the top 0.5 m underlain by sand and gravel. Due to the relatively thin organic-rich layer and lack of geological information for larger depths, we assumed homogeneous thermal and physical properties throughout the 30 m column disregarding any heterogeneity. The model was run for a total of 6 years of data, of which the first 3 years until October 2013 are used as spin-up, and the last 3 years until December 2016 were used for our analysis. Figure 1c shows three optimized model runs and the observed data at a depth of 80 cm, illustrating the match between model and observation. Figure 1d shows the modeled temperature-dependent behavior of the bulk volumetric heat capacity \( (C_v) \) and bulk thermal conductivity \( (\lambda_t) \) (Jafarov et al., 2012) based upon the equations in Table 1.

![Figure 1](image_url)

**Figure 1.** (a) Shows a selection of the observed temperature data at the Qinghai-Tibet Plateau with indications for characteristic freeze-thaw phases, (b) active layer depth interpolated from the measured data set, (c) comparison of observed and modeled temperature for the optimal parameter combinations of the error measures, and (d) modeled volumetric heat capacity and thermal conductivity.
3.2. Error Measures

The error measures RMSE, KGE and Russell’s error are used to evaluate the model performance. RMSE is defined in Equation 2 and is calculated using the observed temperature \( T_{\text{obs}} \) and modeled temperature \( T_{\text{sim}} \), where an RMSE closest to 0 indicates the best performing model:

\[
\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (T_{\text{sim}(i)} - T_{\text{obs}(i)})^2}
\]  

(2)

KGE is calculated using Equation 3 (Knoben et al., 2019), which is a combination of correlation between observation and simulation (\( r \)), standard deviation (\( \sigma \)) and bias calculated with the mean of the simulation and observation (\( \mu \)). A KGE < 0 indicates that the mean of the observed temperature \( T_{\text{obs}} \) better represents the observation than the modeled temperature \( T_{\text{sim}} \), a KGE of 1 indicates the best performance (Gupta et al., 2009):

\[
\text{KGE} = \frac{1 - \frac{3}{2} \sqrt{1 - r^2} - \sigma_{\text{obs}}/\sigma_{\text{sim}} - \mu_{\text{obs}}/\mu_{\text{sim}}}{1 - \frac{3}{2} \sqrt{1 - r^2} + \frac{1}{\mu_{\text{sim}}/\mu_{\text{obs}}}}
\]

Table 1
Numerical Model Parameters

| Parameter | Description | Parameter value |
|-----------|-------------|-----------------|
| \( \phi \) | Porosity, (–) | Variable 0.05 to 0.55<sup>a</sup> |
| \( \lambda_w \) | Thermal conductivity water, (W/m K) | 0.6 |
| \( \lambda_i \) | Thermal conductivity ice, (W/m K) | 2.14 |
| \( \lambda_s \) | Thermal conductivity solid, (W/m K) | Variable 0.05 to 1.175<sup>b,c,d</sup> |
| \( \lambda_t \) | Bulk thermal conductivity, (W/m K) | \( \lambda_t = \phi(S_w \lambda_w + (1 - S_w) \lambda_i) + (1 - \phi) \lambda_s \) |
| \( C_w \) | Specific heat water, (J/kg/K) | 4,182 |
| \( C_i \) | Specific heat ice, (J/kg/K) | 2,060 |
| \( C_s \) | Specific heat solid grains, (J/kg/K) | Variable 525 to 1375<sup>b,d</sup> |
| \( C_v \) | Bulk volumetric heat capacity, (J/m<sup>3</sup> K) | \( C_v = \phi(S_w C_w \rho_w + (1 - S_w) C_i \rho_i) + (1 - \phi) C_s \rho_s \) |
| \( \rho_w \) | Density water, (kg/m<sup>3</sup>) | 1,000 |
| \( \rho_i \) | Density ice, (kg/m<sup>3</sup>) | 920 |
| \( \rho_s \) | Density solid grains, (kg/m<sup>3</sup>) | 2,650 |
| \( L_i \) | Latent heat of fusion, (J/kg K) | \( 333.4 \times 10^3 \) |
| \( S_w \) | Water saturation curve, (T) | \( S_w(T) = 1 - S_{w\text{res}} \exp(-(T - 273.15)/W) + S_{w\text{res}} \) |
| \( S_{w\text{res}} \) | For T > 0 °C, (T) = 1 |
| \( S_w \) | For T < 0 °C, function of (T) |
| \( S_{w\text{res}} \) | Residual saturation, | 0.05 |
| W | Fitting parameter for freezing function | 0.15 |

<sup>a</sup>H. Zhao et al. (2018), <sup>b</sup>Dissanayaka et al. (2012), <sup>c</sup>Abu-Hamdeh and Reeder (2000), <sup>d</sup>Mustamo et al. (2019), <sup>e</sup>Romanovsky and Osterkamp (2000), <sup>f</sup>Putkonen (1998).
The \textit{Russell} error is unique in the way that it evaluates two different properties, the phase error between two signals and the magnitude error, which are synonymous for the correlation and standard deviation (Rokaya & Kim, 2018; Russell, 1997). The \textit{Russell’s magnitude} error ($\varepsilon_m$) is calculated using Equation 4 and the \textit{Russell’s phase} error ($\varepsilon_p$) using Equation 5:

$$
\varepsilon_m = \sin(m) \log_10(1 + |m|)
$$

(4)

$$
\varepsilon_p = \frac{\cos^{-1}(p)}{\pi}
$$

(5)

where $p$ and $m$ are calculated using Equation 6 and Equation 7, respectively:

$$
p = \left( \frac{\sum_{n=1}^{N} T_{obs(n)} T_{sim(i)}}{\left( \sum_{n=1}^{N} T_{obs(n)} \right) \left( \sum_{n=1}^{N} T_{sim(i)} \right)} \right)
$$

(6)

$$
m = \left( \frac{\sum_{n=1}^{N} T_{obs(n)}^2 - \sum_{n=1}^{N} T_{sim(i)}^2}{\left( \sum_{n=1}^{N} T_{obs(n)}^2 \right) \left( \sum_{n=1}^{N} T_{sim(i)}^2 \right)} \right) \left( \frac{\sum_{n=1}^{N} T_{obs(n)} T_{sim(i)}}{\left( \sum_{n=1}^{N} T_{obs(n)} \right) \left( \sum_{n=1}^{N} T_{sim(i)} \right)} \right)
$$

(7)

The \textit{Russell’s comprehensive} (combined) error ($\varepsilon_c$) is a combination of the phase and magnitude error (Equation 8). The \textit{Russell’s phase} is bound by a scale from 0 to 1 and the magnitude error is scaled so that an order of magnitude difference is approximately equal to 1, and is therefore equal to the worst phase error. The combined comprehensive error $\varepsilon_c$ thus has roughly the same scale, with a value of 1 being considered as the worst performance (Russell, 1997):

$$
\varepsilon_c = \frac{\pi}{4} \left( \varepsilon_m^2 + \varepsilon_p^2 \right)
$$

(8)

In this paper, reference to the \textit{Russell’s error} refers to the comprehensive error.

3.3. \textit{Future Scenario}

To investigate the effect of the optimal \textit{RMSE}, \textit{KGE} and \textit{Russell} errors on 100 years predictions of active layer depth, we used a second 1D model and impose a hypothetical scenario of QTP surface warming at the surface boundary. This second 1D model was adjusted to have a domain depth of 100 m and a bottom boundary flux of 0.065 W/m$^2$, which is in the range of geothermal heat fluxes inferred for the QTP (Wu et al., 2010). A shallow fixed temperature bottom boundary condition could lead to an excess of heat storage in the subsurface, therefore a heat flux for $T_{bottom}$ ensures that the development of the permafrost thaw depth over a 100 year period is not limited by a fixed bottom value (Stevens et al., 2007). The time series of imposed surface temperature, $T_{top}$, is based upon the observed 5 cm ground temperature as used in the first model but extended to cover a period of 100 years. The observed data set was used since it contains seasonal variability, mimicking real-world conditions. The IPCC scenarios project an average temperature increase in the Arctic between 2 and 9 °C in 2100 (Anisimov et al., 2007). The $T_{top}$ boundary has a gradual linear temperature increase of 0.05 °C/year (Nan et al., 2005). The model initial conditions were created using a steady-state model and are identical for all of the models, subsequently, a transient model ran over 100 years for the three parameter combinations.
4. Results

Figure 2a shows the variability of fit considering the three parameters \((C, \lambda, \phi)\) for the RMSE error. The parameter space shows a complex interplay in performance determined by the sensitivity of the model fit for each parameter. KGE and Russell parameter spaces show similar behavior. Figure 2b shows the sensitivity of the model for each parameter, keeping the other two parameters fixed at their optimal value. The final column in Figure 2b summarizes the optimal parameter combinations. The optimum RMSE parameter space has high volumetric heat capacity and porosity, whereas the optimal KGE and Russell errors have more comparable optimum parameter values. KGE and Russell both have comparable values for volumetric heat capacity, and the same optimum values for thermal conductivity and porosity. For both the RMSE, KGE and Russell’s error, a change in volumetric heat capacity results in only a very small change in error (Figure 2b). However, variations in thermal conductivity and soil porosity have a much stronger impact on the error between observation and model, indicating a higher sensitivity. The optimal values indicated with the dots all have a local minimum or maximum, indicating that the applied parameter space covers the required range.

The fit varies between observed temperatures and simulated temperatures for the optimized parameter values for each error analysis. Each model accurately simulates the observed temperature data up to 80 cm (Figure 1c). Yet gradually toward 200 cm depth, a mismatch up to 0.5 °C occurs between observed and simulated temperatures for certain time periods. When reviewing the small-scale dynamics (Figure 1c), observed temperatures show more variability in temperature over a greater range compared to the simulated data. At depths of 80–200 cm, the observed temperature variations are smaller compared to large near-surface temperature fluctuations, and the model more accurately captures these dynamics. When investigating the timing of the onset of thawing and associated water-ice phase transition, a short time lag appeared between the observations and the model. At 80–200 cm, observed freezing occurs slightly before the simulated freezing.

Figure 3a shows the simulated temperatures of the hypothetical 100-years future prediction for the models with the lowest RMSE, KGE and Russell’s error. There are clear differences in timing when temperatures switch from sub-zero freezing conditions to positive temperatures. The total period of the phase transition, when temperatures are in the zero curtain period (mushy-zone) and show little change, varies between the optimized models. Figure 3b shows the 100 years model forecast of the active layer depth based upon three optimal parameter combinations from Figure 3a. The seasonal active layer signal is presented as a smoothed yearly (maximum) active layer depth. The initial 40 years (1) show a slowly deepening active layer for all three models. After 40 years (2), the active layer appears to drastically increase in depth for all
models and the once stable permafrost appears to collapse with steep thawing rates. The active layer depth for the Russell and KGE error starts to increase first and shows an average thawing rate of 0.11 and 0.09 m/year when the slope is stable (2). The RMSE error active layer depth lags about 15 years behind Russell and KGE with a comparable increase in active layer depth of 0.10 m/year after 60 years. This time-lag is the time before the two models achieve the same thawing depth. The active layer has developed into a supra-permafrost system, with a perennially thawed aquifer below the active layer which will not refreeze completely in winter. Overall there appears to be a period with a stable active layer, followed by a gradual increase in active layer depth, succeeded by a period of strong active layer development.

5. Discussion and Conclusion

A satisfactory agreement between modeled and observed temperatures was found close to the surface, but a temperature mismatch developed for increasing depth. Clearly, in reality, there is heterogeneity in subsurface thermal properties, as a result of stratification in the active layer. Organic matter content and porosity vary with depth, with higher organic matter contents in the upper 50 cm which could act as an insulator, and lower content at depth (H. Zhao et al., 2018). Influence from the surface-atmosphere boundary such as snow cover can be excluded as a reason for the mismatch since the models were forced with the observations at 5 cm depth, where complex surface boundary interactions are implicitly part of the model. The mismatch between data and model is mainly visible during Phase 4, when temperatures increase during summer, not during freezing. Similarly, Albers et al. (2020) observed that the thermal parameters of their numerical permafrost model are more sensitive close to the surface and during summer time, as this is the time when the active layer is most developed. The temperature mismatch between 100 and 200 cm depth is likely caused by active layer stratification and the statistical method by which the optimal parameter set was determined. By averaging the calculated errors over depth, the model porosity is also averaged over the entire profile, whereas in the field the porosity is variable with depth. The optimal porosity value better represents the top of the profile, given the sensitivity of the porosity, a small change in porosity at depth impacts the modeled temperature substantially. Future modeling efforts could improve model performance by including more layers into the system, at the cost of overall uncertainty due to the doubling of parameters.

The optimal parameter values found in our study agree with ranges reported in the literature. H. Zhao et al. (2018) found average $\phi$ values of 0.25 (−) at a depth of 50 cm for the same region at the QTP. Luo, Jin, He, et al. (2018) observed a thawed summer soil moisture content of 35% at 80 cm depth, which is what

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**Figure 3.** (a) Shows the temperature development at four depths for the optimal parameter combinations determined with the RMSE, KGE and Russell error measures for the 100-years scenario. (b) shows the interpolated active layer depth based upon the optimal parameter combinations.
would be expected in a fully saturated soil with a $\phi$ of 0.35 (−) and is in the same range as the optimal $\phi$ from the RMSE and KGE / Russell parameter combination. A measurement campaign by Chen et al. (2020) used an empirical relation based upon the volumetric moisture content to calculate the bulk thermal conductivity ($\lambda_b$) and different soil fractions to calculate the bulk heat capacity ($C_v$) at two locations around the measurement site at the QTP. The bulk heat capacity ($C_v$) during the cold and warm season varied between $1.4-2.4 \times 10^5 \text{ J/m}^3 \text{ K}$ and the bulk thermal conductivity ($\lambda_b$) between 0.8-1.3 W/m K. When recalculating the optimal parameter space from our study to bulk values using the equations in Table 1, $C_v$ varies between 1.82 and $1.94 \times 10^5 \text{ J/m}^3 \text{ K}$ and $\lambda_b$ between 1.0 and 1.2 W/m K for temperatures above 0 °C, which is in the same range. The thaw rates between 0.09 and 0.11 m/year that developed over the second half the 100 years model period are of similar order with a QTP averaged thaw rate of 0.07 m/year observed by Wu et al. (2012).

The three parameters varied during the study, $C_v$, $\lambda_b$, and $\phi$ have different effects on model sensitivity. Model sensitivity for a change in $C_v$ is low and $\lambda_b$ and $\phi$ have higher model sensitivities. $\phi$ controls the amount of liquid water and ice in the pore space, and thereby the required latent heat of fusion during phase transition. When temperature gradients during freeze-thaw transitions are limited or of a short time period, there can be a deficit in the energy supply to complete the phase transition. Consequently, the pore water will remain in the "mushy zone", and will not completely thaw. The sensitive nature of $\phi$ and $\lambda_b$ affects the accuracy of long-term predictions, as is demonstrated with the hypothetical 100 years scenarios. Over the 100 years model period (Figure 3), the differences between the optimal parameter combinations are visible. There are small differences in thawing rate and a 15 years time-lag developed that is, likely the result of the larger/lower $\phi$ for the latter models. Due to a higher $\phi$, the water content increases, subsequently requiring more energy to complete the phase transition. Over the first period (1), the active layer depth is deeper for KGE and Russell because they have a lower $\phi$ and thus lower water content. As a result, the active layer thaws to a deeper depth during the summer period compared to the RMSE parameter combination. The time lag of 15 years can be considered very significant because it impacts the timing of active layer thaw and activation of solute transport from thawing permafrost. This highlights that model error uncertainty has a high impact on the overall uncertainty of active layer development models.

The QTP is an area of interest subjected to ongoing research related to active layer thaw and permafrost degradation. Permafrost thaw modeling is frequently used to study the evolution of the active layer (Qin et al., 2017; Z. Sun et al., 2020). This research demonstrates a method to analyze observed data to determine the porosity and thermal properties of the active layer. This helps to improve model parameterization and increases our understanding of the timescale of active layer thaw and the uncertainties involved. Our method is capable of acquiring satisfactory thermal properties from direct subsurface temperature observations. The presented method is well suited to be applied to other permafrost sites with predominantly conductive heat flow, due to the straightforward 1D nature of the model setup. However, careful consideration should be taken with respect to snow melt or precipitation infiltration, as this can cause advective heat flow. Our approach reduces the need for intensive laboratory research by using temperature observations to determine the soil-specific thermal properties, which could be applied to other permafrost temperature observations on the QTP and across other permafrost areas. This also avoids the need for thermal property estimation based upon surface data and empirical relations. The analysis showed that next to the model parameters, the error measures also have a sensitivity range, which is usually not considered in permafrost modeling studies, but do have a large impact on long-term active layer predictions. Sensitivity analysis of the error measure should therefore become an integral part of the overall system sensitivity analysis. As shown in this study, over longer periods, substantial differences in active layer thawing rate and depth prediction arise, due to the use of the various error measures. The QTP active layer is a tipping point system, as once a certain threshold is exceeded, the system changes to a new state and cannot return easily to the old state. Once the QTP active layer thickness exceeds the threshold, the active layer system collapses, and livelihoods will be affected due to potentially irreversible environmental changes. A well founded understanding of permafrost thaw, timing, and uncertainty is therefore of vital importance to understand the sensitivities of the system and inform communities about the implications for their livelihoods.

**Data Availability Statement**

Observed temperature data are made available by Luo, Jin, He, et al. (2018).
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