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Reply on RC1

Carlotta Brunetti et al.

Author comment on "Probabilistic estimation of depth-resolved profiles of soil thermal diffusivity from temperature time series" by Carlotta Brunetti et al., Earth Surf. Dynam. Discuss., <https://doi.org/10.5194/esurf-2021-68-AC1>, 2022

Below you can find the original Reviewer's comments and our replies (authors' comments) highlighted in *italics*.

The manuscript describes an interesting and timely study that applies the Bayesian method to the measured at multiple depth temperature time-series to estimate/recover thermal diffusivity. The method and implementation are sound. My main concerns: The choice of the model. The thermal model worked well for the examples shown in this study (i.e. when we are dealing with temperatures above 0°C). However, it was shown in many studies that applying the classical thermal equation described in this study does not capture the full temperature dynamics in permafrost-affected soil (Romanovksy et al., 2000). The effect of the unfrozen water is an essential factor that needs to be accounted for.

Dear reviewer,

Thank you very much for taking the time to review the manuscript and provide your valuable feedback.

Based on the reviewers' comments, we realized that we did not explain clearly enough the reasons why in this study we are using a heat-conduction-based model without representation of advection and latent heat process, its advantages and limitations, and why we used it in an Arctic environment. We clarified this in the revised manuscript.

The thermal model we are using (heat-conduction-based model without representation of advection and latent heat process) is only adequate and used to simulate heat transfer during periods of time when conduction dominates advection and when temperature remains well above 0°C (above 0.5°C in our study). This means that in our case study in the Arctic environment, we only apply this model to time periods when the soil is entirely unfrozen along the probe and when rain events are minimal. We agree that estimating thermal diffusivity during freeze-thaw processes would require us to account for the effect of unfrozen water (Romanovksy et al., 2000). Still, we do not intend to do that in our study.

The main reason that guided our choice of using the heat-conduction-based model is that in many situations, hydrological boundary conditions are difficult to assess. Indeed, using a more complex model (including advection and/or latent heat) would require to force or parametrize the model with information that is much more difficult to collect than temperature. For example, rain precipitation and its partitioning between surface flow and

infiltration is a major source of uncertainty that we would need to account for if we simulate soil moisture variations. Similarly, representing freeze-thaw process would require to assess first the water content in unfrozen soil and thus would require to measure or estimate several parameters. While we are aware that a few studies have been estimating thermal conductivity by including the freeze-thaw process, they have generally assumed the total water content constant, used additional datasets from intensive sites, or made assumptions given the site hydrological conditions (e.g., full saturation) (Jafarov et al., 2014, Nicolsky et al., 2010). Still, in our study we aimed at developing a method that can be applied at locations where only temperature data are present, and where soil water saturation and porosity is variable. Thus, we decided to use a heat-conduction-based model without representation of advection and latent heat process to reduce the number of parameters to be estimated or constrained (and hence the likelihood of non-uniqueness of solutions) while limiting the applicability of our model to time periods when the soil is unfrozen and the heat advection is limited (i.e., dry period considered for our case study in the Arctic environment).

Finally, it can be noted that our approach involves repeating the estimation of thermal diffusivity with a moving time-window that:

1- is as short as possible in order to enable the estimation of thermal diffusivity during time-windows devoid of significant water fluxes (e.g., advection) not represented in our heat-conduction-based model, as well as the detection of advection processes that may occur intermittently e.g., caused by percolation events. In this study (Section 4), we showed that when such events take place the misfit between the model and the data is expected to increase, and thus the moving time-window approach can be used to evaluate when our model lack hydrological process representation.

2- does enable the detection of changes in thermal diffusivity over time, presumably linked to changes in water content

Overall, while we agree that our model does not represent all the complexity of hydrological processes, we believe this approach is pragmatic for many applications, and reliable when applied under the above-mentioned conditions.

How the Bayesian approach used in this study is different from the variational approach when the gradient is explicitly/implicitly calculated to find the next iteration?

The bayesian inference problem can indeed be solved using various methods among which the Markov chain Monte Carlo (MCMC) method (as applied in our study) or the variational approach.

The main difference is that the MCMC method approximate the target (posterior) distribution via sampling schemes (i.e., no model is assumed) whereas variational inference finds the best parametrized ensemble of distributions that represent the target one (i.e., a model is assumed).

*Generally, MCMC methods are more accurate than variational approaches but require more computational resources. (More info can be found here: Blei, David M., Alp Kucukelbir, and Jon D. McAuliffe. "Variational inference: A review for statisticians." *Journal of the American statistical Association* 112.518 (2017): 859-877).*

Please extend the discussion on estimating thermal diffusivities at or near 0oC and estimating thermal diffusivities during time periods when the gradient sign changes from positive to negative.

In our study, we use only temperature time series that are at all depths above 0.5°C (soil entirely unfrozen). Indeed, close to 0°C latent heat transfer occurs due to water freezing and melting processes. In this study, we infer thermal diffusivity only in time-windows in which temperature is above 0.5°C in order to not violate our conductive heat transfer model assumption.

By applying our inference approach under various temperature fields, we observed that the change in sign of the temperature gradient (i.e., similar to the case in Fig 1 in the paper) does not cause any issue in the reliable inference of thermal diffusivity by itself. However, if the temperature gradient changes sign very slowly over time then it likely implies low temperature gradients over long period of time which will degrade the inference of the thermal diffusivity.

In Section 3.4. it was not clear how the optimal number of sensors had to be selected. In the Discussion, the authors mentioned the effect of low gradients between temperature time-series makes it hard to estimate diffusivity. This finding is also consistent with studies by Jafarov et al., (2014; 2020). What is the best way to proceed in the case of a low gradient? Is it better to exclude those chunks of data from the method? How can this method be used at the design stage to build temperature probes that could capture optimal temperatures signals (i.e. no low gradient signals)?

Thank you for mentioning Jafarov et al., (2014; 2020) that we have now cited in the discussion section.

In our view, there are two possible way to proceed in the case of low temperature gradients:

*remove the time windows with low temperature gradients from the analysis
increase the length of the moving time window and/or decrease the depth at which infer thermal diffusivity (e.g., for the application of our method in the Teller site in Alaska, we decided to increase the time window from 7 to 10 days and to investigate thermal diffusivity up to 0.85 m instead of 1m). We improve the discussion on the time windows length in the revised manuscript.*

Thank you for your interesting question on the creation of the temperature probe to optimally capture temperature signals.

Given the high variability of the temperature gradients overt time and of soil composition, it might be difficult to think of a probe at the design stage that is generally optimized for low gradient signals. Based on the synthetic experiments implemented in section 3.4, we were however able to identify some important aspects to consider at the design stage of temperature sensors such as:

- having more sensor closer to the soil surface where temperature signal has the highest content of information (e.g., diurnal and seasonal fluctuations).*
- using temperature probes (i.e., sensors placed on the same support as used in this study) instead of discrete temperature sensors placed manually in the subsurface, which implies higher uncertainty in the distance between sensors.*
- the more vertically heterogeneous is the soil under study the more important is to have many sensors to ensure a vertical spatial resolution that capture as much as possible the soil layering*
- collecting very high-accuracy measurements, which require optimization in sensor accuracy, sensor spacing and the all system accuracy. Improving system accuracy is still challenging, yet critical depending on the environmental conditions.*

In addition, we provided values that one can consider as a starting point to design a probe optimal for their study. Indeed, we concluded that, under the environmental conditions with median diurnal fluctuations $\geq 1.5^{\circ}\text{C}$, temperature gradients $> 2^{\circ}\text{C m}^{-1}$, temperature sensors with a level of noise $< 0.02^{\circ}\text{C}$, a bias defined by a standard deviation of 0.01°C or less, and a positioning accuracy of a few millimeters or less (i.e., temperature probe) is needed to ensure reliable thermal diffusivity estimates up to 1 m deep.

We have clarified all this in the revised manuscript.

Minor concerns:

Consider simplifying the title and removing "and uncertainty quantification" because, in the end, you recovered diffusivity from temperatures not from UQ. Consider including UQ

into the search words for the paper.

We modified the title to "Probabilistic estimation of depth-resolved profiles of soil thermal diffusivity from temperature time series"

L121-122 It was mentioned that diffusivity depends on soil moisture. It is not clear how water content is accounted for in the eqn. 2.

We will add a sentence explaining this more clearly. Indeed, the fraction of water in soil affects the density, the specific heat capacity and the thermal conductivity. Thermal diffusivity depends on all these three quantities and therefore it is indirectly affected by the soil moisture.

L421-422 The moving-time window. Jafarov et al., (2014) found that 30 days moving average filter worked the best when applied to changing over time snow thermal conductivity. Will 30 days average window here? If not, why?

The optimal length of the time-window depends on the data information content and the site-dependent nature of hydrological processes. Comparing our time-window strategy to the 30 days moving average filter in Jafarov et al., (2014) does not seem adequate to us. Jafarov et al. (2014) study, though very interesting in many aspects, seem to use a time-window to constrain the variability of snow thickness. We think this goal is quite different from our objective when using a moving time-window.

In our study, we used a time-window length as short as possible in order to limit the influence of hydrological processes (e.g., water fluxes not represented in the heat-conduction-based model) but sufficiently long to reliably infer thermal diffusivity. Moreover, the shorter the time-window the higher the temporal resolution at which thermal diffusivity changes can be detected. In our study, we use 7 days (10 days for the study at Teller site) moving time-window. However, we show that 4 days are sufficient under certain environmental conditions (Section 3.1, Figure 1).

In conclusion, include the caveats about the model (does not account for soil moisture), the method (will it fail with low gradient data), and how choosing different moving average windows will affect the estimated diffusivity.

We will add sentences in the introduction, method and discussion sections to state more clearly the reasons why we use a heat-conduction-based model and the related limitations of our approach. Concerning the impact of choosing different lengths for the time window, we will clarify it in Section 3.1, depicted in Figure 1 and discussed in Sec. 6.