

Response to reviewers' comments to the manuscript:" The effect of sediment thermal conductivity on vertical groundwater flux estimates, MS number: hess-2018-210

First of all the authors would like to thank the two anonymous reviewers for the encouraging and useful comments! Based on the suggestions we believe that we managed to address all concerns of the reviewers and generally improve the clarity of the manuscript.

Please note that the references to page, line and figure numbers in the corrected manuscript refer to the revised manuscript submitted together with this response.

Response to Referee #1:

General comments: The paper presents an evaluation of the influence of vertical thermal conductivity variability on the estimates of vertical GW-SW exchange fluxes. The analysis and conclusion of the paper are based on depth-resolved measurements of saturated sediment thermal conductivities (k_e) and the inverse modelling of observed sediment temperatures.

The paper is generally well written and presents original data. The authors discuss their findings in the light of the numerous other studies in the field of heat as a natural hydrologic tracer. While there are no ground-breaking new results, the paper contributes to further constrain the uncertainties associated with thermal conductivity estimation in heat tracing studies.

Specific comments:

p.3. l.12-14. This sentence is redundant to the one in p.2. l. 31.

Action: Sentence at p.3, l. 12-14 removed.

Consider to remove/rephrase Section 4.1. The reported thermal conductivities of partially <0.6 W/m/K are lower than those of pure water. Could this be attributed to accidentally unsaturated conditions? Otherwise such low values seem very unlikely if not physically impossible in saturated sediments. The low values should be discussed in Section 5.2.

The thermal conductivity of sediments is influenced by the density, moisture content of the sediments, also the salinity of pore water and the content of organic matter in the sediment material (Abu-Hamdeh and Reeder, 2000). During the field measurements some of the sediment cores became unsaturated (p.5., l. 4-5) and sediment thermal conductivity values were therefore removed from the analysis.

Both at the lagoon and at the stream site organic matter and plant debris was also occasionally trapped in the sediment columns, close to the sediment surface at shallow depths. Thus it is assumed that in some cases organic matter decreased sediment thermal conductivity. Pooling all thermal conductivity values together, four measurements gave a thermal conductivity below $0.73 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$ and three of these measurements were made at the stream site which is known to have organic debris also deeper in the sediment column (Sebok et al., 2014). As neither unsaturated conditions, nor organic sediments were visually identified for these samples and the measurement error was within the chosen limits of the

study ($0.05 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$), the authors did not find any rigorous reason to remove these values from the validated measurements.

Action: As Section 4.1 only presents our validated results we chose not to change the text and discuss the issue in Section 5.2.

Text in Section 5.2 was rephrased, now including: *‘At the stream site unusually low sediment thermal conductivity values between 0.55 and $0.65 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$ were observed. These values are clearly outliers in their respective measurement depths (Fig. 2). However, as the sediment core did not become unsaturated, nor the measurement error was too high to discard the measurement, it is assumed that sediment organic matter resulted in such a low thermal conductivity value which was previously shown to be occasionally present also deeper in the stream sediments (Sebok et al.,2014).’* (p.9., l. 27-31.)

Section 4.2. and Fig. 3. The measured temperature-depth profiles, including the cases with poor model fits, seem to reasonably represent a steady state case with upward water flow. I wonder if the depth of the domain (only 1m) and the selected lower temperature boundaries are really appropriate. My impression is that the boundary conditions are too rigid to provide a good fit. For example: in Fig. 3 - P1 the lower temperature boundary seems too low. Maybe extend the model domain to greater depths or use the lowest temperature measurements as boundary condition.

In answering this comment we would like to refer to each field site separately. At the stream site, at the high discharge zone the upward groundwater flux is high enough for reaching stable groundwater temperatures at 1 m depth below the streambed surface as also presented by field measurements in other studies (Karan et al., 2013; Jensen and Engesgaard, 2011), thus in case of the stream site we do not think it is necessary to change the depth of the lower temperature boundary condition. Especially as the RMSE of the temperature profiles is between 0.02 and $0.32 \text{ }^\circ\text{C}$, while the measurement accuracy was $0.2 \text{ }^\circ\text{C}$.

At the lagoon site upward groundwater fluxes are lower, thus stable groundwater temperatures will not be reached at 1 m depth below the lagoon surface where we set the lower temperature boundary. We have however several reasons to maintain the temperature boundary condition at 1 m depth below the lagoon surface:

- **As already discussed in the manuscript text (p. 8, l. 28 – p. 9, l. 1), in the low flux lagoon site assuming only vertical flow conditions may not be correct as wave action can also induce a temporary horizontal flow component in shallow depths. Moreover, the diurnal variations in air temperature are more pronounced in the upper part of the temperature profiles (for a more precise description please refer to the response given to Referee #2). If we use the measured temperatures at 0.5 m depth as a boundary condition, we can only fit the model to temperature data collected up to 0.35 m depth, which is shallow enough to be exposed both to a horizontal flow component and diurnal temperature variations. For this reason we would argue against moving the model boundaries up to the temperatures measured at 0.5 m depth.**
- **In the lagoon at greater depths density-driven flow also induces a strong horizontal groundwater flow component by the movement of the saline wedge that varies depending on the season and recharge conditions. Based on field data, Müller et al. (2018) estimated the depth of the density driven flow at approx. 2 m below the lagoon surface, thus moving the model boundary deeper than 1 m would also introduce additional uncertainty to the flux estimates.**

- Sediment temperature was measured at 7 locations (0, 5, 10, 15, 20, 35, 50 cm depth) below the lagoon surface. Using the temperatures measured at 0 cm and 50 cm depth as boundary conditions would also mean that we only can evaluate the fit between observed and simulated data at 5 depths, where four of the measurement points are only 20 cm below the lagoon surface. As this area is the most affected by the diurnal temperature changes, we think that we also need the temperature data at 50 cm depth to have a more robust flux estimate and also to include as much of the measured data in the estimation process as possible.
- Selecting the temperature boundary condition at 1 m below the lagoon bed is also a good way to minimize boundary effects, while using temperature data at 0.5 m depth would introduce an even more rigorous boundary condition, thus influence flux estimates in a higher degree. As an example at profile P1 using the temperatures measured at 0.5 m depth below the surface as a lower boundary condition would increase the obtained flux values in such a degree that they are not realistic anymore. For profile P1, this would result in an increase from 0.17 m/d to 0.35 m/d. Having several years of field work experience at the site (Haider et al., 2014; Duque et al., 2016) the authors carried out numerous temperature profile-based and seepage meter based flux estimates which never showed such high flux values at the lagoon.
- Our most important argument about using the presented boundary condition is that our aim with the manuscript was to conceptualize the effect of using various, even vertically heterogeneous distributions of measured sediment thermal conductivity and study their effect on flux estimates. Using the same temperature boundary conditions at the same depth provides a common background to all measured temperature profiles at the respective field sites. We feel that using different temperature boundary conditions for profiles measured 10-15 minutes and 1 m apart would not provide for a stable background for comparison. Furthermore, our interest lies in the differences between flux estimates within individual profiles using different sediment thermal conductivities, instead of describing the spatial variability of flux estimates within different temperature profiles. For the within-profile comparison, results are representative if the same boundary conditions are used for all cases of different sediment thermal conductivities. Thus, we think that irrespective of the RMSE of the profiles, the change in the RMSE while using different sediment thermal conductivities is sufficient to make conclusions about the effect of using different sediment thermal conductivities on vertical flux estimates.

In order to test the effect of the depth and temperature of the boundary condition on the flux estimates, we reanalyzed profile P1 from the lagoon which had the one of the worst RMSE values of all profiles in this study assuming the average sediment thermal conductivity measured in the profile.

- Using the sediment temperature measured at 0.5 m depth resulted in a flux estimate of 0.35 m/d with an RMSE of 0.37 °C. Thus the authors would argue against using the measured sediment temperature at 0.5 m depth as a lower boundary condition due to the unreasonably large flux estimate
- Using a common, assumed groundwater temperature of 11.5 °C at different depths, the following flux estimates and RMSE were obtained with an analytical solution:

Depth of stable groundwater temperature (m)	Flux (m/d)	RMSE (°C)
0.5	0.15	1.00
1	0.16	0.77
1.5	0.16	0.75
2	0.16	0.75
3	0.16	0.75
4	0.16	0.75
5	0.16	0.75

Thus assuming a constant groundwater temperature at greater depth than 1 m would not considerably improve the RMSE of the profile, while the flux values stay constant. Raising the constant temperature boundary to 0.5 m would on the other hand increase RMSE and result in unreasonably high fluxes.

Based on both the theoretical considerations and the results obtained in profile P1 we would argue against changing the depth of the boundary condition as in a greater depth the RMSE improves slightly, but more uncertainty is introduced in the profiles by entering the zone of the density-driven flow dynamics.

No action

p.7.1.18 and following. k_e and vertical water fluxes (q_z) are related. In steady-state 1D, homogeneous conditions there should be functional relationship between q_z and k_e . I suggest to present the results along the theoretical relationship. Then it would also be possible to evaluate/visualize the effect of heterogeneous vs homogeneous k_e .

There is certainly a functional relationship between k_e and q_z (Figure 1, in response) which is clearly visible assuming a homogeneous distribution of k_e through the vertical sediment column. Our intention in the manuscript however was to present the different flux values that can be obtained by using actual k_e measurements within one single profile within real field settings rather than a theoretical range of potential k_e values. This way the emphasis of the study is not on how much the fluxes change when assuming a range of k_e values, but the fact that such a large range of k_e values could be measured within the profiles thus highlighting the importance of selecting an appropriate k_e value for flux calculations.

No action

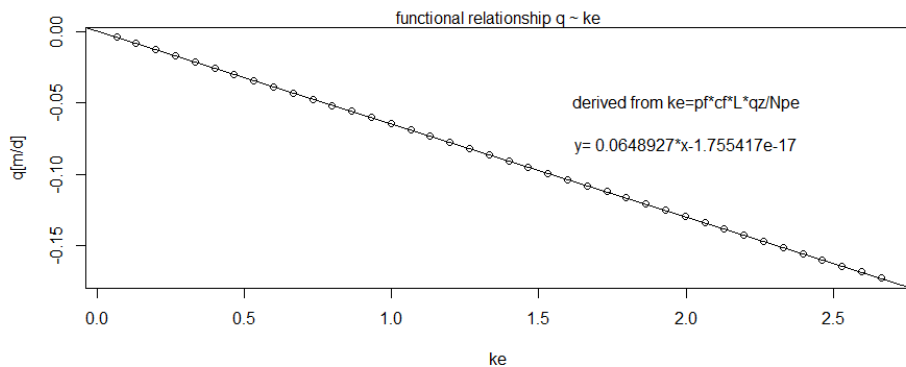


Figure 1: The functional relationship between k_e and q derived from the Peclet number.

p.8. 1.21-28. Maybe the limited spatial resolution of the measurements calls for a geostatistical approach, similarly to generation hydraulic conductivity fields, to come up with spatially continuous scenarios of k_e . Maybe briefly discuss this option.

This is an interesting point made by the Referee. In the text (p.8 1. 24-25) we highlight that the vertical natural variability in the sediments may be higher than what we sample. We have several reasons, why we did not include geostatistical approaches creating e.g. variograms in the manuscript:

- i) From a geostatistical point of view only an appropriate sample size can create meaningful variograms. Eventhough our data is of relatively high resolution compared to previous studies, there are still too few datapoints in vertical direction to generate meaningful vertical variograms.**
- ii) To overcome such a problem we could bin all observations together. But that would require similar sedimentation conditions and spatially continuous data. Both of these requirements are violated by the three different measurement sites as well as the different depositional environments: stream environment, open lagoon, protected lagoon bay.**

At the same time we attempted a geostatistical approach in case of the peat profiles of the lagoon.

- i) From the test variogram, the calculated range was very short (Figure 2, in response), on the scale of 0.2 m. Hence, we would argue that geostatistical approaches similar to hydraulic K field generation would be largely biased by the few vertical datapoints collected**

Moreover its application to the present environment may be inappropriate. As this natural environment is characterized by large heterogeneity occurring due to small-scale faunal activity (worm or crab activity etc.), rooting of plants disturbing sediment structures or erosional events caused by storm wave activity rearranging the natural settling conditions expected in near coastal zones. Furthermore, all those factors influence the natural setup on a very short temporal scale (especially tidal and wave actions).

No action

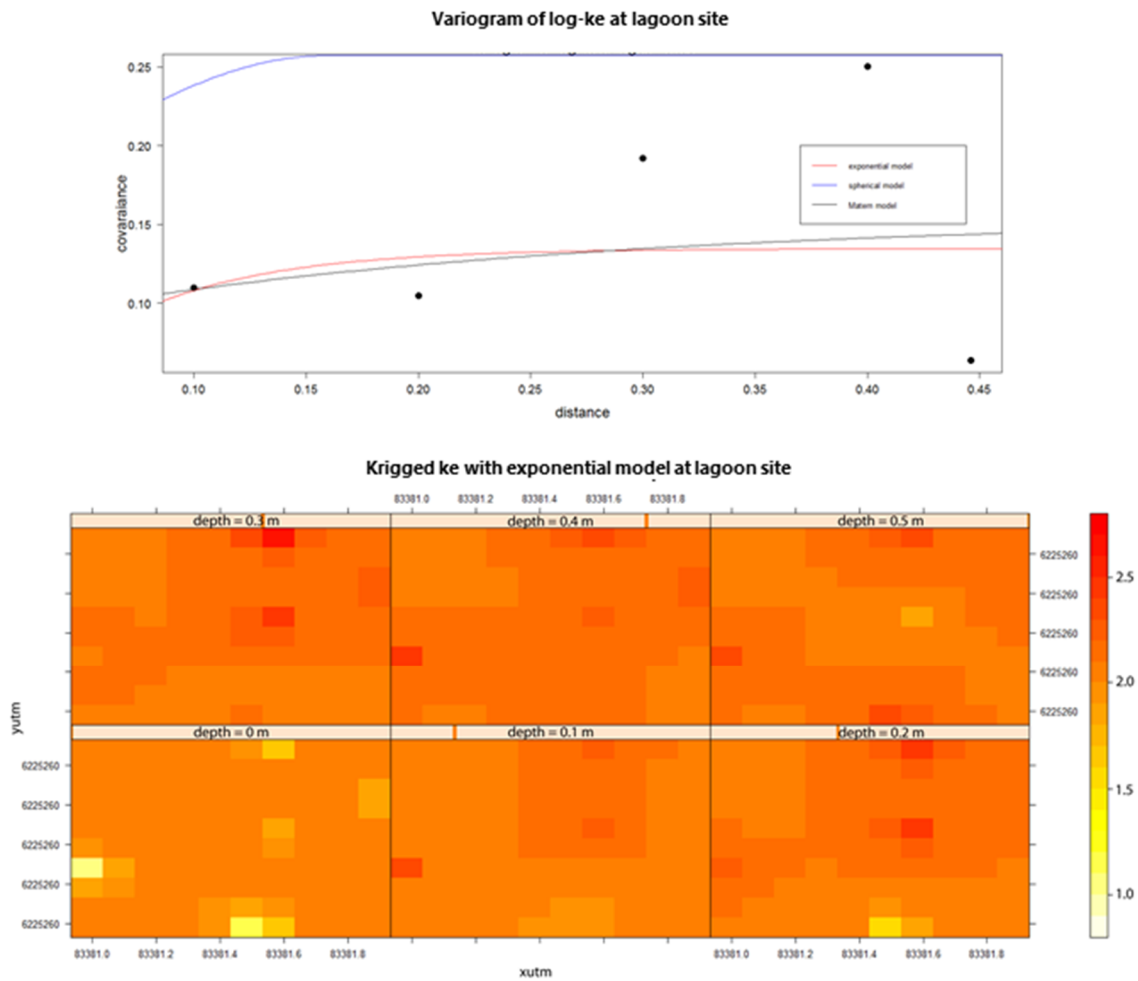


Figure 2 Geostatistical exploration of k_e at the lagoon sites. Upper panel shows the variogram of the log values of k_e . A very short range of 0.2m is established and thereby a low vertical spatial relation is achieved. After a distance of 0.2 m no spatial relation can be established between the values. The lower panel shows kriged horizontal k_e surfaces at different depths using the exponential model. Here a large variability of values in each separated depth can be seen. However, due to the few datapoints per depth the resulting spatial statistics may be highly biased.

p.9. 1. 21. Does k_e really increase with grain size? If porosity and the sediment material do not change one would expect k_e to be constant (if one assumes that k_e of the water-sediment mixture can be modelled by the volume fractions and the thermal conductivities of water and sediment grains). An alternative explanation for the observation could be that the shallow sediments are less consolidated and have a higher porosity which could explain the lower thermal conductivity. I think, as porosity was not measured, the porosity-dependence should be mentioned and discussed.

We agree with the Referee that sediment thermal conductivity k_e depends on porosity, which is related to grain size and packing conditions.

Action: The manuscript text was rephrased to: *“An explanation for this could be that measurements in this study were also made at other depths below the SWI, where thermal conductivity values show a generally increasing trend with depth. This is likely to reflect a transition from finer, less consolidated sediments of higher porosity to coarser, more consolidated sediments of lower porosity.”* Page 9 line 20-23

Technical comments:

p.5 l.4. better "within" instead of "in"

Action: Changed

Figure 1. Add a scale to the insets in b and c

Scale added to the insets.

Figure 4. Cases should be "thermal conductivity" not diffusivity

Figure inscription corrected.

References:

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