

Estimating groundwater discharge to surface waters using heat as a tracer in low flux environments: the role of thermal conductivity

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Abstract:

Analytical modelling of heat transport was used to address effects of uncertainty in thermal conductivity on groundwater–surface water exchange. *In situ* thermal conductivities and temperature profiles were measured in a coastal lagoon bed where groundwater is known to discharge. The field site could be divided into three sediment zones where significant spatial changes in thermal conductivity on metre to centimetre scale show that spatial variability connected to the sediment properties must be considered. The application of a literature-based bulk thermal conductivity of $1.84 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$, instead of field data that ranged from 0.62 to $2.19 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$, produced a mean overestimation of 2.33 cm d^{-1} that, considering the low fluxes of the study area, represents an 89% increase and up to a factor of 3 in the most extreme cases. Incorporating the uncertainty due to sediment heterogeneities leads to an irregular trend of the flux distribution from the shore towards the lagoon. The natural variability of the thermal conductivity associated with changes in the sediment composition resulted in a mean variation of $\pm 0.66 \text{ cm d}^{-1}$ in fluxes corresponding to a change of $\pm 25.4\%$. The presence of organic matter in the sediments, a common situation in the near-shore areas of surface water bodies, is responsible for the decrease of thermal conductivity. The results show that the natural variability of sediment thermal conductivity is a parameter to be considered for low flux environments, and it contributes to a better understanding of groundwater–surface water interactions in natural environments. Copyright © 2015 John Wiley & Sons, Ltd.

KEY WORDS temperature; temperature probes; thermal conductivity; Ringkøbing Fjord; groundwater flux

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INTRODUCTION

The interaction between groundwater and surface water is attributed enormous importance in scientific studies with its interplay of hydrological (Winter *et al.*, 1998), biological (Baird and Wilby, 1999), chemical (Winter *et al.*, 1998) and environmental (Hayashi and Rosenberry, 2002) factors. Currently, this impacts management of water catchments and drives political regulations (European Union Framework, 2000). Fluxes resulting from head gradients, whose magnitude is governed by hydraulic conductivity, can trigger biogeochemical processes as a result of the exchange and mixing of waters with different physical and chemical properties when either groundwater flows into surface water or surface water encroaches an aquifer (Krause *et al.*, 2009). This subject encompasses a wide range of physical environments from rivers, lakes, ponds, reservoirs to seas, and various techniques and

methods are available to study and quantify the systems (Kalbus *et al.*, 2006). Groundwater–surface water interaction occurs at different spatial ranges, but the exchange between both water bodies is mostly located in a variable-sized fringe near the shore line of, e.g. lakes or lagoons (McBride and Pfannkuch, 1975; Genereux and Bandopadhyay, 2001), where the application of similar study methods is possible.

However, the variability of the magnitude of groundwater fluxes to or from surface water due to the natural heterogeneity of sediments (e.g. Kishel and Gerla, 2002; Sebok *et al.*, 2015), the hydrological conditions like rainfall/infiltration or changes in water levels/gradients (e.g. Rosenberry *et al.*, 2013; Karan *et al.*, 2014) and the different time and measurement scales are still a great challenge for research. One solution in these circumstances is the collection of a large amount of data in order to have a complete overview of the study area characteristics like distribution of sediment properties and how it affects spatial variation in fluxes. Here, the use of temperature as a natural tracer emerges as a method with high potential, because of the ease and low cost of data collection, and the

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recent technical improvement in data collection and analysis (Anderson, 2005; Constantz, 2008). Rau *et al.* (2014) divided heat tracer research into studies of fundamental heat transport, method development and comparisons, spatial and temporal variability of fluxes and limits and capabilities of the method. From this list, it can be noted that even if the study of heat as a tracer has a long tradition, there are still fundamental questions to be answered, among others, the limitations of the method and the improvement of temperature data interpretation.

Vertical temperature profiles in beds of streams, lakes or lagoons represent the gradual change in groundwater temperature when approaching the sediment bed of a surface water body. The shape of the profile is due to heat exchange processes (convection and conduction) with the surrounding sediments and surface water. This technique has been extensively used to study groundwater–surface water interaction, for example, by temperature envelope analysis (Taniguchi, 1993; Duque *et al.*, 2010), by matching observations with analytical solutions of the heat transport equation (Schmidt *et al.*, 2006) or by numerical models (Schornberg *et al.*, 2010). Depending on the spatial scale of the relevant processes, temperature profiles of 10s of metres (Taniguchi *et al.*, 1999) or centimetre scales (Anibas *et al.*, 2009) have been used. Temperature profiles can readily be a qualitative indicator of the flux direction, e.g. if a river is gaining or losing (Silliman and Booth, 1993) or be used in a quantitative way to estimate the flow gained or lost to or from a surface water body (Constantz *et al.*, 2002). The development of analytical solutions (Suzuki, 1960; Bredehoeft and Papadopulos, 1965; Stallman, 1965) and matching calculated and observed profiles has been the preferred way for the estimation of fluxes. Recently, the analysis of temperature time series has led to a branch of studies based on the differences in amplitude and time lag between groundwater and surface water temperature oscillations (Hatch *et al.*, 2006; Keery *et al.*, 2007; Lautz, 2012). These methods require the monitoring of thermal changes for longer periods in order to calculate fluxes based on the difference in temperature time series measured at different depths. On the contrary, the use of temperature profiles punctually on time provides a snapshot of the temperature distribution that could be a practical field method but requires near steady state boundary conditions and, thus, should avoid periods with abrupt weather changes (Schmidt *et al.*, 2006; Anibas *et al.*, 2009).

Vertical temperature profiles can be obtained with temperature probes in wells measuring at multiple levels or with sensors located at certain depths that monitor periodically. The main advantage of quantifying fluxes with temperature probes resides in the potential to obtain a reliable estimate of the fluxes by simple analytical solutions (Schmidt *et al.*, 2006; Anibas *et al.*, 2009),

preferable at multiple locations covering a significant surface area and with low-cost fieldwork equipment and computing time. It is generally not required to drill expensive wells or have sensors installed during long periods, and it provides a quick quantification of the flux, when the restrictions in the application of the method (like steady state 1D flow) are fulfilled. The variability of groundwater fluxes could be higher spatially than temporally; hence, measurements at many locations may be needed.

The analytical solutions require defining temperature boundary conditions in both groundwater and surface water and the sediment properties such as thermal conductivity. The thermal conductivity is the property that describes the conductive heat transport capacity of a material. In most studies, this value is obtained via laboratory studies, based on the thermal bulk properties of sediment and water (Ronan *et al.*, 1998; Constantz *et al.*, 2002; Anderson, 2005; Keshari and Koo, 2007; Anibas *et al.*, 2009; Ferguson and Bense, 2011). Stonestrom and Constantz (2003) showed that the variability in sediment thermal conductivity is less than the variability in hydraulic conductivity (and therefore likely the flux). The impact of uncertainty in thermal conductivity on the estimation of fluxes is therefore generally believed to be low. Nevertheless, in near conduction-controlled systems (low fluxes), uncertainty in thermal conductivity values may lead to significant uncertainty in flux estimations. A few works have tried to assess the impact that this parameter may have on flux calculations (Constantz *et al.*, 2002), for example, by a sensitivity analysis (Keshari and Koo, 2007), but generally, it has not been the main objective of most studies. One of the main reasons is that it is rarely measured in the field (Shanafield *et al.*, 2011), often leading to the pragmatic assumption of homogeneity using laboratory-derived values. Many other parameters and circumstances of applying the simple analytical solutions have been intensively studied on the other hand, such as the impact of non-vertical (Schornberg *et al.*, 2010; Ferguson and Bense, 2011) and non-uniform flow components (Cuthbert and Mackay, 2013), the effect of transient/steady-state conditions (Anibas *et al.*, 2009; Vandenbohede and Lebbe, 2010b), the impact of sensor spacing and accuracy (Vandenbohede and Lebbe, 2010b; Shanafield *et al.*, 2011; Soto-López *et al.*, 2011), the influence of geological heterogeneity (Schmidt *et al.*, 2006; Schornberg *et al.*, 2010) and effects of diurnal temperature oscillations (Stallman, 1965; Lapham, 1989). But, spatial variability in thermal properties of the sediments is usually a minor topic even if the uncertainty in discharge has been attributed to changes in thermal properties in some cases (Anderson, 2005; Vandenbohede and Lebbe, 2010a).

A few studies have explored the impact of variation in thermal properties on flux estimation, and most of them

are based on theoretical approaches or modelling exercises. Taniguchi (1993) pointed out that an increase in the thermal properties by 5% would result in increased groundwater flux of 10.3%, while a decrease of 5% would reduce groundwater flux of about 9.8%. Constantz *et al.* (2002) used a Monte Carlo analysis with 400 simulations to find a 50% uncertainty in the percolation rate due to changes in thermal conductivity. Keshari and Koo (2007) performed a numerical sensitivity test of the thermal diffusivity (thermal conductivity divided by bulk density and heat capacity) leading to changes of $\pm 18\%$ in the flux. Shanafield *et al.* (2011) evaluated the impact of thermal diffusivity on discharge with Monte Carlo analysis assuming a thermal conductivity between 0.8 and $2.5 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$. All these studies emphasize the impact of the thermal properties on flux estimation, but little work has been performed to test and evaluate these methods under various field conditions (Rau *et al.*, 2010). Another common assumption is the homogeneity of the thermal properties even if the studies cover areas of 100s of square metres. It is well known that in rivers, lakes and coastal areas, the sediment properties can change greatly over short distances. This has been quantified with modelling approaches (Schmidt *et al.*, 2006; Schornberg *et al.*, 2010), and Karan *et al.* (2014) found that streambed fluxes were equally sensitive to variation in both the hydraulic and thermal conductivity across a 40 m^2 stream bed. Nevertheless, seeking a simple scenario, most studies assign a homogeneous thermal conductivity in the entire study area for estimating flux. Accordingly, the objectives of this work are the following:

- (i) Determine homogeneity of the thermal conductivity in lagoon bed sediments.
- (ii) Compare the effect of using standard literature values for thermal conductivity as opposed to *in situ* field measurements on estimated groundwater fluxes from modelling of *in situ* measured temperature profiles.
- (iii) Assess the impact of the natural variability in thermal conductivity on flux calculations.

A field study area was selected at the west coast of Denmark, where groundwater flows into a coastal lagoon as has been shown by previous studies (Kinnear *et al.*, 2013; Haider *et al.*, 2014).

STUDY AREA

Ringkøbing Fjord, a coastal lagoon in the west coast of Denmark (Figure 1A) (latitude $55^\circ 58' 40'' \text{N}$, longitude $8^\circ 14' 21'' \text{E}$), offers near-ideal conditions for the application of temperature tracing methods as water depth is shallow ($\sim 0.5 \text{ m}$). It is therefore possible to carry out measurements up to tens of metre offshore after which the deeper parts of the fjord is reached. According to previous studies, the mean water depth of the fjord is 1.9 m (Ringkøbing Amt, 2004), and groundwater discharges to the lagoon along the eastern shore line (Kinnear *et al.*, 2013; Haider *et al.*, 2014). The lagoon has an area of 300 km^2 containing brackish water (5–15%) due to its connection with the sea through a sluice and the seasonal discharge from the Skjern River (yearly average of $50 \text{ m}^3/\text{s}$) (Figure 1B) (Kirkegaard *et al.*, 2011). Annual mean precipitation and evaporation are 1050 mm and 630 mm, respectively (Kirkegaard *et al.*, 2011).

The surface geology is dominated by Pleistocene fluvio-glacial sand that can include layers of lower permeability materials such as silt or paleo-channels with higher hydraulic conductivity. The lagoon bed is covered with small ripples of sand without detectable visual changes in the sediment composition further off-shore. As in most coastal areas, the vegetation adapted to brackish water grows in the proximity of the shore line and covers the sandy sediments. The area surrounding the lagoon has a gentle topography, mostly flat with small scale undulations due to old dunes now covered with vegetation. The hydrogeological characteristics of the area are still under investigation, but preliminary results indicate an unconfined aquifer of at least 12 m thickness based on the analysis of the borehole archive data of the Geological

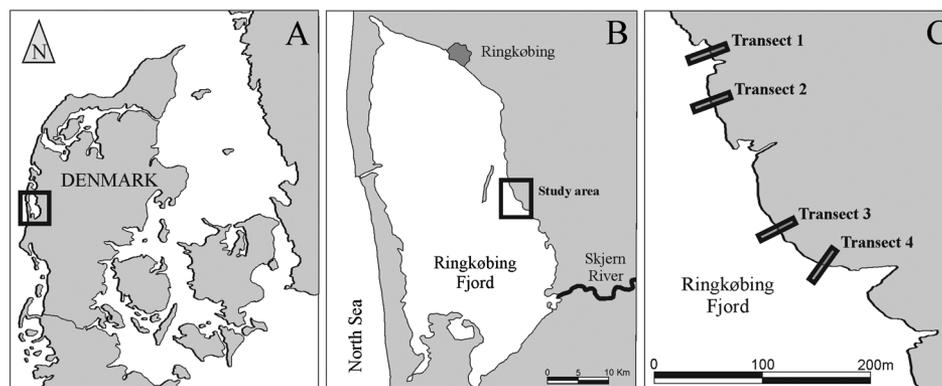


Figure 1. Location of Ringkøbing Fjord (A), the study area (B) and the four studies transects (C)

Survey of Denmark as well as drilling campaigns. In the coastal fringe, the water table is reached at a short distance (<1–2 m) beneath the surface, and horizontal hydraulic gradients close to the shore are 0.005–0.010 estimated based on water levels in wells on land and lagoon stage.

The measurements of this field study were accomplished along a 300-m long stretch of the shore divided into four transects of 20- to 25-m length perpendicular to the shore (Figure 1C). Having four transects and measuring over several seasons during a year provides observations of a wider range of variability of spatial and temporal fluxes. According to theoretical studies of groundwater–surface water interaction in homogeneous environments, most of the discharge occurs near the shore line with an exponential decrease offshore (McBride and Pfannkuch, 1975; Winter *et al.*, 1998).

METHODS

Multiple vertical sediment temperature profiles were measured with a 0.5-m long temperature probe along with the determination of *in situ* sediment thermal properties at approximately the same location. Both were linked through the use of the analytical solution proposed by Bredehoeft and Papadopoulos (1965) that estimates the vertical groundwater flux on the basis of the thermal conductivity of the sediment and the temperature profile data.

The temperature distribution in the lagoon bed was measured with a vertical probe consisting of 10 temperature sensors (thermocouples with an accuracy of $\pm 0.2^\circ\text{C}$) located at several depths from the lagoon bed (0, 2.5, 5, 7.5, 10, 15, 20, 25, 35 and 50 cm; i.e. the top sensor was placed right at the sediment–water interface). The measurements were acquired after a stabilization period of 10 min based on a field experiment where the temperature was measured during 2 h every 15 min in the same location with changes of 0.01°C after 15 min and 0.02°C after 1 h. This indicates that, in term of practical reasons, thermal equilibrium was achieved in less time, and the chosen time period ensures the stability of the temperature. The temperature data were obtained during three surveys in May, August and October of 2012 with more than 150 temperature profiles collected in total. Each of the four transects contained 8–20

measurements positioned approximately at similar locations (for a schematic layout see Figure 2).

The thermal conductivity of the sediment was determined using a KD2 pro with the SH-1 sensor (Decagon Devices, Pullman, WA, USA). The sensor's accuracy is $\pm 10\%$ at thermal conductivities between 0.02 and $2\text{ W m}^{-1}\text{ }^\circ\text{C}^{-1}$. The measurements rely on the heating of a needle and the detection of the heat pulse in a second needle after a period of 30 s to detect how the heat disperses in the media by that time. A total of 60 readings were collected during a 2- to 8-min collection period and averaged giving the bulk thermal conductivity as well as the measurement error for that location. The bulk thermal conductivity of a porous material depends on the properties of the solid phase and its structure as well as the water content and its properties. The thermal conductivity of solids varies largely from $8.4\text{ W m}^{-1}\text{ }^\circ\text{C}^{-1}$ in quartz minerals to $0.25\text{ W m}^{-1}\text{ }^\circ\text{C}^{-1}$ for organic matter (De Vries, 1963). Water usually shows values close to $0.6\text{ W m}^{-1}\text{ }^\circ\text{C}^{-1}$, while air thermal conductivity is $0.025\text{ W m}^{-1}\text{ }^\circ\text{C}^{-1}$. A resume of values for soil types or porous media and individual phases indicates a great variety of possible values depending on the composition of the sediment and porosity (Stonestrom and Constantz, 2003). Bulk thermal conductivity or effective thermal conductivity is calculated as follows (Woodside and Messmer, 1961):

$$K_o = K_w^n * K_g^{1-n} \quad (1)$$

where n is porosity (or moisture content in unsaturated material), K_w is the thermal conductivity of the fluid and K_g is the thermal conductivity of the grains/rock. In this work, the term thermal conductivity of sediments is referred to as the bulk thermal conductivity because the sediment is composed of solid particles and voids (porosity), and all the samples are fully saturated.

The thermal conductivity was measured directly in the study area where the natural conditions cannot be controlled. The values could therefore be affected by upward groundwater flow heating or cooling the needle, but, considering that the discharge fluxes in the lagoon bed are in the range of a few cm/d (Results section), the water movement during a period of minutes will not change the results substantially. A similar device has been already

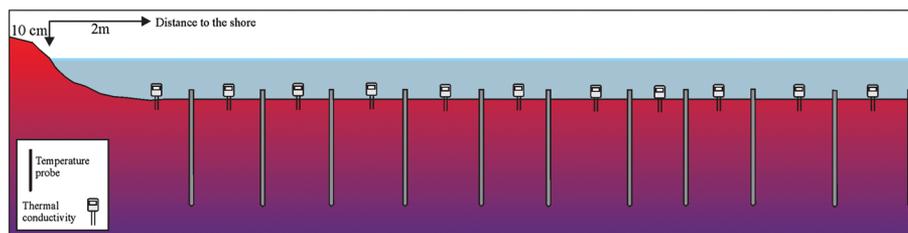


Figure 2. Structure of the transects with temperature probes and sediment thermal conductivity measurements

applied successfully in the calculation of groundwater fluxes in laboratory studies (Mamer and Lowry, 2013) and in the field (Sebok *et al.*, 2014). The thermal conductivity of lagoon sediments was measured in one survey during October 2013 along the four transects at approximately each metre to cover the area previously surveyed with the temperature probes (Figure 2). Also, three experimental plots of 1 m² were selected in areas along the transects, where thermal conductivity was relatively homogeneous (in transects 1, 3 and 4) to characterize the range of lateral variability in sediment thermal properties within the distance separating the temperature probes. In each plot, 13 measurements were carried out with spacing around 15–20 cm.

The analytical solution of the 1D steady heat transport equation presented by Bredehoeft and Papadopoulos (1965) has been recommended for gaining conditions (Shanafield *et al.*, 2011) such as observed in this area:

$$T(z) = T_s + (T_g - T_s) \frac{\exp[N_{pe}(z/L)] - 1}{\exp[N_{pe}] - 1} \quad (2)$$

where $T(z)$ is the temperature (°C) at depth z (m), T_s is the surface water temperature (°C) at the sediment–water interface, T_g is the temperature of the groundwater (°C) at a given depth L (m) and N_{pe} is the Peclet number showing the ratio of convection to conduction:

$$N_{pe} = \frac{q_z \rho_f c_f L}{K_e} \quad (3)$$

where q_z is the vertical fluid flux (ms⁻¹), ρ_f is the density of the fluid (kg m⁻³), c_f the specific heat capacity of the

fluid (Jkg⁻¹°C⁻¹) and K_e is the bulk thermal conductivity (W m⁻¹°C⁻¹).

The only unknown in Equation (3) is the vertical flux, q_z , which is then estimated by fitting the simulation results from (2) to each observed temperature profile (Figure 3). Here, a manual calibration was chosen. The advantage of the manual fitting over the automatic is that isolated errors or inconsistencies in the measurements can be excluded in the fitting procedure by taking into account the shape of the temperature profile and disregarding local effects or even sensor inaccuracy.

The values of the parameters considered in the analytical solution were obtained from different sources based on their physical properties (Table I). The specific heat and density of water were considered fixed values even if the density could be slightly higher because of the mixing with brackish lagoon water. Because the location of the measurements is close to the shore, density was assumed to be dominated by discharging fresh groundwater. Groundwater temperature was expected to oscillate between 8 °C and 11.5 °C based on the thermal stability of groundwater reported in previous studies (Arriaga and Leap, 2004) as well as in Denmark (Karan *et al.*, 2013). The difference in deeper groundwater temperature between October and May–August was attributed to the heating of the system at the end of the summer season. The surface water temperature was obtained from the top sensor in the temperature probes located at $z=0$. The surface water temperature changed between each measurement because of diurnal changes, wind conditions and depending on the weather of the monitoring day. For this reason, they were averaged for each survey to obtain a mean daily value that

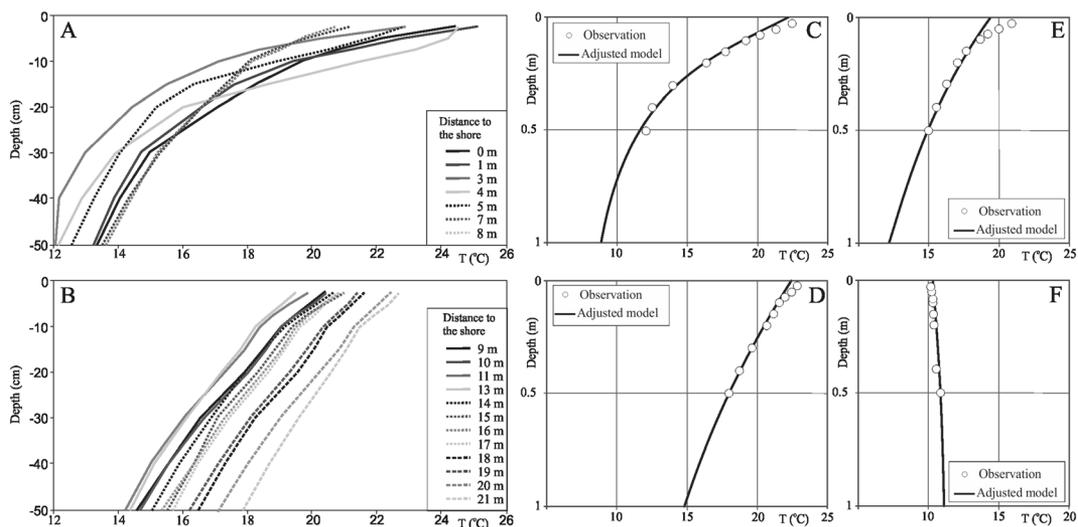


Figure 3. Temperature profiles for transect 1 (May, 2012). (A) Closer to the shore (0–8 m) and (B) more offshore (9–21 m). Good fit of analytical solution to observations for (C) near shore profile (transect 3, May) and (D) off-shore profile (transect 1, May). (E) Example of poor match in the top of near-shore profile (transect 1, August) and (F) example of small differences between temperatures and thus boundary conditions in groundwater and surface water for October (transect 1)

Table I. Parameter values for the analytical solution

Parameter	Symbol	Unit	Value
Density of the fluid	ρ_f	kg m^{-3}	1000.8
Specific heat capacity of the fluid	c_f	$\text{J kg}^{-1} \text{ } ^\circ\text{C}^{-1}$	4192
Distance to stable groundwater T	L	m	5
Groundwater temperature (May)	T_g	$^\circ\text{C}$	8
Groundwater temperature (August)	T_g	$^\circ\text{C}$	8
Groundwater temperature (October)	T_g	$^\circ\text{C}$	11.5
Surface water temperature (May)	T_s	$^\circ\text{C}$	22.35
Surface water temperature (August)	T_s	$^\circ\text{C}$	19.34
Surface water temperature (October)	T_s	$^\circ\text{C}$	10.31
Effective thermal conductivity	K_e	$\text{J m}^{-1} \text{ s}^{-1} \text{ } ^\circ\text{C}$	a, b, c

^a Standard value assigned commonly in previous studies,

^b Values measured in the field,

^c Max and min detected in experimental plots in the field, see text

could be used for all profiles. This can lead to difficulties in fitting the analytical solution to observed temperature values close to the sediment–water interface. Thus, temperature data from 20 cm and deeper in the lagoon bed was prioritized over the ones located closer to the surface (Conant, 2004). This was also a way to exclude the effect of daily temperature oscillations that can influence temperature measurements in the top 20 cm below lagoon bed (Goto *et al.*, 2005; Schmidt *et al.*, 2006). A general refinement of boundary conditions (temperatures of groundwater and surface water) could improve the fitting with the analytical solution, but this is limited by the data availability and the relevance it would have on the fluxes. For example, the uncertainties produced by the error in the temperature measurements ($\pm 0.2 \text{ } ^\circ\text{C}$) were estimated based on a change of the groundwater temperature from $8 \text{ } ^\circ\text{C}$ to $7.8\text{--}8.2 \text{ } ^\circ\text{C}$ for transect 1 in August. The modification of this boundary condition leads to mean changes in upward flux of $\pm 0.017 \text{ cm d}^{-1}$ with a maximum of $\pm 0.050 \text{ cm d}^{-1}$ for 12 temperature profiles. Whether this is relevant depends on the flux magnitude and the precision needed. The thermal conductivity was measured directly in the field and used in the analytical solutions depending on the experiments in small plots as well as the distance to the shore.

RESULTS

The sediment temperature profiles all show a gradual change from the lagoon bed to the deeper locations, with more uniform temperatures at 50-cm depth than close to the lagoon bed (lower temperature than at the lagoon bed in May and August and opposite in October), indicating upward groundwater flux (Taniguchi, 1993). A few

temperature profiles from May in transect 1 are presented in Figure 3 as examples of data showing two characteristic patterns depending on the distance to the shore. Closer to the shore of the lagoon (Figure 3A), the profiles display a concave downward trend that it is common in areas where groundwater seeps into surface waters. The temperature range is representative for Danish conditions such as lakes (Sebok *et al.*, 2013) or rivers (Jensen and Engesgaard, 2011). In these studies, the temperature of groundwater was around $8 \text{ } ^\circ\text{C}$, some metres below the lake/stream bed corresponding to the mean annual atmospheric temperature in Denmark. The concave downward trend shifts into a linear trend at locations further offshore (Figure 3B) indicating an even more uniform temperature changes over the whole profile. Usually, a trend like this is interpreted as a reduction of the upward groundwater flow, where the dominant heat transport process is conduction and not advection/convection (Land and Paull, 2001; Anibas *et al.*, 2009).

The observations and the analytical model agree well in most of the cases for the near shore profiles (example in Figure 3C) and more off-shore profiles (example in Figure 3D). There are exceptions with a poorer fit, which often can be explained by the choice of boundary conditions in the analytical solution. For example, one of the most common mismatch between the model and the observations was found close to the lagoon bed (Figure 3E). This is linked to the selected lagoon water temperature boundary condition as well as the changes produced by the daily oscillation of lagoon water temperatures affecting lagoon bed temperatures down to 10- to 20-cm depth. These effects have been reported in other study areas (Goto *et al.*, 2005; Schmidt *et al.*, 2006). Therefore, during the manual adjustment, a good match with the deeper measurements was prioritized. Also, for the measurements during October (Figure 3F), the differences between groundwater and surface water temperatures are smaller, and hence, small inaccuracies in temperature measurements or assignment of boundary conditions may lead to greater uncertainty in the calculated flux.

The measured thermal conductivities show a common pattern in the four transects (Figure 4) in zones of variable length (a few metres for transect 2 and more than 10 m for transect 4). In the first zone, close to the shore, values are lower than $1 \text{ W m}^{-1} \text{ } ^\circ\text{C}^{-1}$, followed by a gradual increase (transect 2 and 3) or an abrupt rise to close to $1.5 \text{ W m}^{-1} \text{ } ^\circ\text{C}^{-1}$ that is assigned to zone 2. In this zone, the pattern is irregular with sudden increases and decreases in thermal conductivity. Finally, the zones located more offshore (from 10 to 20 m) show the highest values (around $2 \text{ W m}^{-1} \text{ } ^\circ\text{C}^{-1}$) with a lower variability. Based on these observations, the transects were divided into three zones (or sediments 1–3) with three types of sediment thermal conductivities.

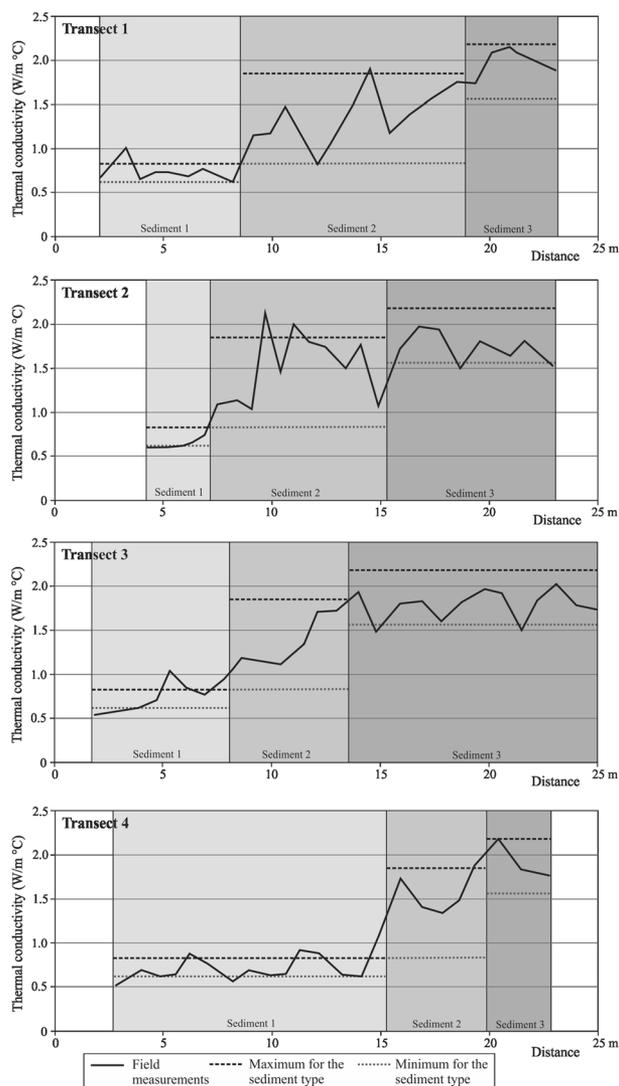


Figure 4. Measured bulk thermal conductivity in four transects. The transects have been divided into different sediment zones of different length (in a transect and between transects) based on the observed patterns. Maximum and minimum values are explained in Figure 6

To compare the effect of assuming a standard homogeneous thermal conductivity based on literature values and the direct measurements in the field, the vertical groundwater flux was calculated by matching the analytical solution to observations changing only the thermal conductivity values for both cases. The assumed thermal conductivity for the standard case was $1.84 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$, a mean value for sandy sediments applied previously in river or lake sediments (De Vries, 1963; Stonestrom and Constantz, 2003; Chen, 2008). The field measurement-based values were assigned according to the three segments defined based on different thermal conductivity patterns and magnitude. A mean value was calculated for each zone: 0.72 , 1.46 and $1.82 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$ for zones 1, 2 and 3, respectively.

The differences between the two flux calibrations decrease when the value of thermal conductivity based on field measurements is close to the standard value (Figure 5). Accordingly, the differences are maximal in the areas closer to the shore (sediment 1) and negligible at the most distant part (sediment 3). Also, the differences are larger when the magnitudes of the fluxes are higher. In Figure 5, it can be observed that the difference between the two calibrations is up to 6 cm d^{-1} in transect 1 for May, which is the location and season with highest fluxes, while the difference is lower, $2\text{--}4 \text{ cm d}^{-1}$, for transect 2 and transect 1 in May and October. These differences can change groundwater fluxes by a factor of 2–3 depending on the assigned thermal conductivity. Nevertheless, as the measurement of the thermal conductivity was not carried out exactly at the same time and location as the temperature profile measurements, and, because both measurements are a point measurement in space, there is the risk that the zonation and the assigned value of thermal conductivity used here are not an entirely accurate representation of the thermal properties of the sediments as local heterogeneity can produce changes at small scales.

With the purpose to test the potential variability of the thermal conductivity in the study area, three experimental plots were selected in each of the three sediment types. The thermal conductivity was measured 13 times in a 1 m^2 area assumed to be representative of the expected variation due to the uncertainty in location of the measurement device (Figure 6). As the temperature probes were installed with a spacing of one metre, this was the distance considered to produce variability in thermal conductivity because of uncertainty in the measurement distance.

The variability of the thermal conductivity measured in 1 m^2 confirms that the three types of sediments assigned along the transects can be considered as having distinct thermal properties (Figure 6). Sediment 1, the one closer to the shore, has the lowest thermal conductivity values and a low variability with minimum and maximum thermal conductivities of 0.62 and $0.83 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$, respectively. Sediment 2 shows a wider range of values, from 0.83 to $1.86 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$, with changes up to $1 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$ over very short distances (15 cm). Finally, sediment 3, located more offshore presents the highest values with a range of 1.56 to $2.19 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$. To check if these ranges are representative, the maximum and minimum values for each of the sediments are shown in Figure 4, where it can be seen that most of the measurements collected within a transect (87%) are included into the ranges based on the experimental plots.

The maximum and minimum thermal conductivities measured in the experimental plots were used to quantify the impact of natural variability on calculating discharge to the lagoon. As the range of observed values is different for each sediment type, three different uncertainty bands

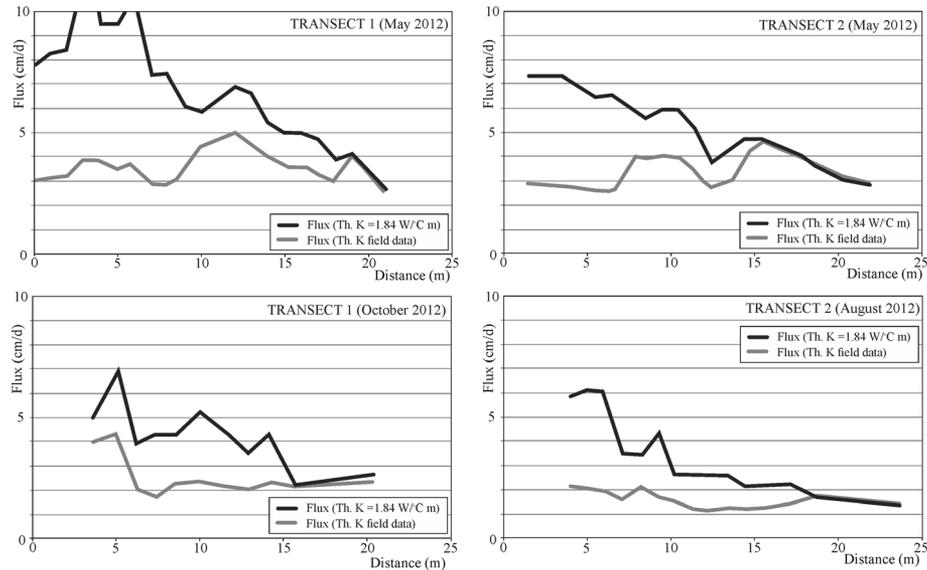


Figure 5. Differences in flux calculated with thermal conductivity usually assigned for sediments in rivers and lakes compared with the fluxes obtained from direct measurements in the field

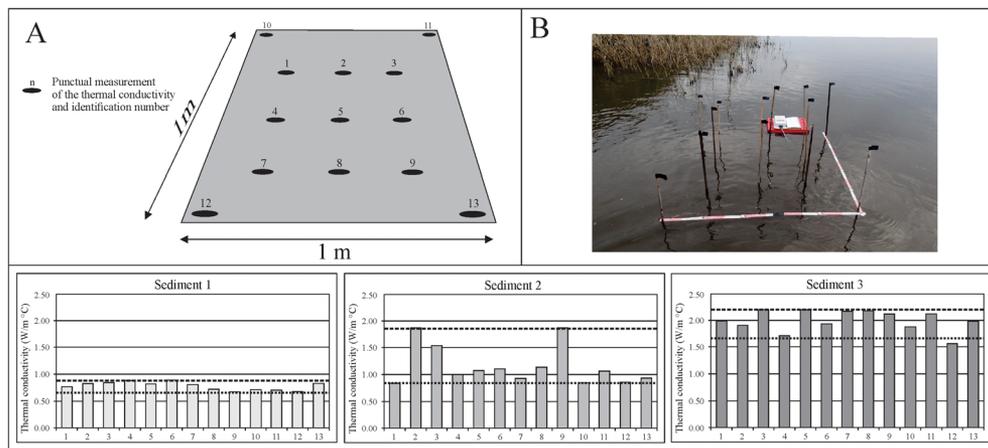


Figure 6. Experimental plot structure (A), field photo (B) and thermal conductivity for each sediment type with marks corresponding to the minimum and maximum thermal conductivities detected in the sediment

are shown around estimated fluxes calculated on the basis of the mean thermal conductivity of the three sediment types (Figure 7). The uncertainty band on fluxes in the first and third sediment type are smaller than in sediment type 2, where a higher uncertainty band is produced by the higher natural variability of the thermal conductivity. The changes in estimated fluxes due to this uncertainty range vary from $\pm 0.5 \text{ cm d}^{-1}$ to more than $\pm 2 \text{ cm d}^{-1}$ from the mean value considering that the mean flux in all zones is around $2\text{--}3 \text{ cm d}^{-1}$. When comparing with fluxes estimated by applying standard values not only a change in magnitude but also distribution is observed. With a standard value of thermal conductivity, most of the transects present a very clear decrease in fluxes from areas close to the shore to areas offshore. With the *in situ* thermal conductivity

values, this pattern is less clear and sometimes difficult to identify because of irregular peaks in fluxes.

The mean estimated flux using mean values of measured thermal conductivity (Figure 6) is 2.61 cm d^{-1} . The mean flux obtained applying the standard value of $1.84 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$ is 4.94 cm d^{-1} , that is, an increase of 2.33 cm d^{-1} , or a potential overestimation of 89%. When considering individual temperature profiles, these differences can be up to a factor of three (8.81 cm d^{-1} in transect 1 in May, distance 3.0 m , Figure 7).

In general, using *in situ* thermal conductivities produce a decrease in the fluxes. Considering all 157 temperature profiles, the reduction in flux is between 34% (3.27 cm d^{-1}) and 61% (1.94 cm d^{-1}) when using the maximum and minimum measured thermal conductivity, respectively

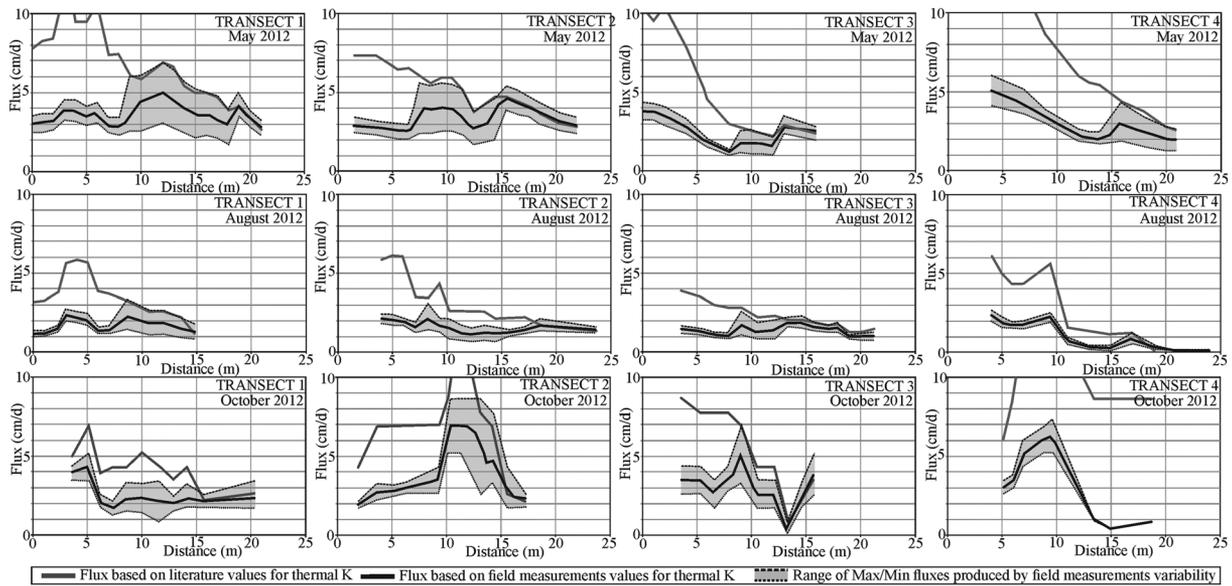


Figure 7. Comparison of fluxes calculated with standard value of bulk thermal conductivity (Table I) and with the minimum, mean and maximum values measured in the field measurements in the four transects and three surveys in May, August and October

(Table II). The flux estimated based on the mean thermal conductivity of all measurements was also lower than when using the standard value. The differences within individual transects indicate that this reduction can be higher with differences of -55% to -69% for the minimum and maximum values measured in transect 4 compared with -23% to -56% in transect 2 (Table II). The seasonal changes in the calculated flux show similar percentages, but with different absolute values. For example, while in August the mean flux applying the standard thermal conductivity of $1.84 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$ was 2.9 cm d^{-1} , and for October 6.3 cm d^{-1} , the flux differences with the maximum and minimum thermal conductivities measured in the field were -39% and -62% and -36% and -62% , respectively (Table II).

Table II. Mean fluxes by transects and seasons and differences between using a standard value for bulk thermal conductivity and the maximum and minimum measured values

	Flux for Th. $K = 1.84 \text{ cm d}^{-1}$	Flux difference with max Th. K measured (%)	Flux difference with min Th. K measured (%)
Average	4.9	-33.8	-60.6
By transects			
Transect 1	5.2	-29.9	-60.1
Transect 2	4.9	-22.6	-55.8
Transect 3	4.0	-32.0	-59.2
Transect 4	5.8	-54.5	-68.6
By seasons			
May	5.8	-30.1	-58.9
August	2.9	-39.0	-61.7
October	6.3	-35.9	-62.4

Th. K , thermal conductivity

DISCUSSION

A reduction of 30% to 60% in estimated groundwater fluxes is a consequence of using *in situ* measurements of thermal conductivities instead of assuming standard values found in the literature. The fluxes using a standard thermal conductivity (e.g. $1.84 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$) can be two to three times higher than fluxes estimated based on field measurements. This change is highly dependent on the magnitude of the fluxes, and it will be more relevant in areas with low fluxes like Ringkøbing coastal lagoon (fluxes on the scale of $1\text{--}5 \text{ cm d}^{-1}$). Nevertheless, this magnitude is relatively frequent in natural environments, with recent studies (Rosenberry *et al.*, 2015) showing an average exfiltration rate to lakes of 0.74 cm d^{-1} . Also, small differences over large areas can have a quantitative impact. A difference of 2 cm d^{-1} along the length of the lagoon interacting with the uppermost aquifer (25 km) in a 20 m wide fringe, would lead to a decrease of $10\,000 \text{ m}^3$ per day.

The differences in fluxes between transects are produced by the different lengths of the three types of sediments occurring in each transect. Similar spatial variability can be considered in other study areas where, depending on the sediment characterization, the comparison of fluxes estimated with measured or standard thermal conductivity values may vary. The differences in this study should be considered as a qualitative indicator of the impact of uncertainty in the thermal conductivity in different sediments as the number of temperature profiles for each type of sediment is different; 67 for sediment 1, 58 for sediment 2 and 32 for sediment 3 in a non-equal proportion for each transect. This affects the calculated mean fluxes values.

The estimated fluxes may be affected by the method applied for measuring the thermal properties. The needle of the KD2 pro was inserted in the sediments to a maximum depth of 10 cm, while in the 1D analytical solution a homogeneous thermal conductivity is assumed along all the sediment profile. In natural environments, a higher proportion of organic deposits and/or less consolidated sediments is usually found in the uppermost layer of sediments. This may generate the underestimation of the thermal properties depending of the thickness of these materials. The vertical changes in thermal properties have been poorly studied so far and have been considered only in a few cases (Wörman *et al.*, 2012) even though it not only affects the magnitude of estimated fluxes but also modifies the shape of the thermal profiles (Su *et al.*, 2006). Additional laboratory studies about the vertical changes in sediment thermal conductivity with sediment columns or with field data collection would help to refine the data and results presented here. Also textural changes, for example, sand becoming finer with depth would lead to a decrease in thermal conductivity (Su *et al.*, 2006). Another source of potential errors is the temperature boundary condition of surface water and groundwater. They could be refined by considering a more detailed description of the natural conditions like distance to the shore, depth of the surface water, seasonal groundwater temperature and wind conditions. This is beyond the scope of this work, where the aim was to highlight the effect of thermal conductivity on groundwater flux estimates.

Based on the geological information available as well as a general overview of the area, the initial assumption of sand as the dominant material in the lagoon bed was reasonable. But, a more detailed field analysis confirmed that the main contrasts in sediment thermal conductivity in all transects (Figure 4) are due to the presence of organic matter reducing the bulk thermal conductivity. This is almost never considered in the application of heat as a tracer even if the thermal properties of this material are well described (Stonestrom and Constantz, 2003) and used in specific studies about peatlands (McKenzie *et al.*, 2007). Sediment thermal parameters usually are assigned considering standard values representing only sand (assuming no presence of organic matter that would cause a reduction in bulk thermal conductivity). Interestingly, the environments where these heat tracer studies were accomplished are rivers, lakes and coastal areas, where vegetation in near-shore areas is common because of plant growth in shallow water and even accelerated by the delivery of nutrients by groundwater (Frandsen *et al.*, 2012). Constantz (2008) pointed out the difficulties of applying this method in lake environments because of the differences in sediments found in lakebeds and streambeds. Our results justify that statement. Nevertheless,

many rivers have layers of organic matter or very fine sediment textures that would lead to a similar reduction in sediment thermal conductivity (Conant, 2004; Wörman *et al.*, 2012; Sebok *et al.*, 2015).

When modelling sediment temperature profiles for estimating groundwater discharge to surface water bodies perpendicular to the shore line, the most common trend would be an exponential decrease from the shore according to field studies and theoretical/numerical modelling studies in homogeneous media (McBride and Pfannkuch, 1975; Lee, 1977; Winter *et al.*, 1998). However, there are cases where this pattern is not detected and where the temperature-based estimation does not match other methods (e.g. see page meter measurements or Darcy calculations). A possible explanation is that changes in sediment thermal conductivity generate these differences as can be observed in the change in spatial pattern of groundwater fluxes at Ringkøbing Fjord (Figure 7). According to calculations with the standard thermal conductivity for sand ($1.84 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$), there is a clear decreasing trend from the highest value in the proximity of the shore to lower values more offshore. With the *in situ* thermal conductivities this trend is less apparent. The pattern is more smooth in many of the transects, and it is also possible to detect different spatial patterns with low fluxes in the proximity of the shore, higher fluxes at 10- to 15-m distance, or irregular trends with high and low peaks in flux (Figure 7). As an example, with the uncertainty bands in Figure 7 in transect 2 for May 2012, there is almost no trend in fluxes moving offshore. In some sections, a short exponential decrease until a certain distance is seen, or with several peaks. Nevertheless, all these possibilities are captured by the natural variability of the thermal conductivity. This range considers the uncertainty produced by small-scale sediment heterogeneity; the fluxes exceeding these margins can point to other reasons that require further study like geological unit changes, preferential flow paths, instrumental errors or environmental conditions changes.

Sediments are naturally heterogeneous at different scales, from the changes of geological units to sediment type changes at centimetre-scale to metre-scale, for example, different ratios of sand-clay or organic matter content. The variability of the thermal conductivity in the experimental plots can be considered as the natural variation associated with the centimetre-scale to metre-scale heterogeneity of the sediments in the study area. Usually all the unconsolidated sediments from clay to gravel are merged in one category of thermal conductivity (Stonestrom and Constantz, 2003). The data collected in this study shows that this natural variability produces, on average along the transects, a change in flux of $\pm 0.66 \text{ cm d}^{-1}$ that represents $\pm 25\%$ of the estimated flux values as consequence of applying the highest or lowest

thermal conductivity obtained in the experimental plots. These differences are intrinsic of the sediment properties, and changes of this magnitude can be expected in natural environments. Taking into consideration spatial-temporal point data (data corresponding to a specific temperature profile), the maximum difference found in the dataset because of the natural variability increases to $\pm 3.02 \text{ cm d}^{-1}$ (October, transect 2, 8.20 m distance) (Figure 7). These calculations show that natural variability in thermal conductivity at centimetre scale induce changes in the flux estimations, but still not as high as the maximum differences produced by using thermal conductivity based on standard literature values instead of field measurements ($+8.81 \text{ cm d}^{-1}$ for transect 1 in May, distance 3.0 m) (Figure 7).

This work represents an investigation of low submarine groundwater discharge and, thus, an environment where heat conduction can be as important as heat convection. The thermal conductivity will therefore play a critical role in estimating exchange fluxes. In a low flux environment, the absolute changes in fluxes because of changes in thermal conductivity are small, but on a relative scale, the changes can be considered significant. Our results highlight the broad importance of measuring the thermal conductivity and assessing the spatial heterogeneity in order to quantify groundwater discharge with temperature measurements.

CONCLUSIONS

The application of different thermal conductivity values based on literature or field measurements leads to quantitative and qualitative changes in flux estimates and distribution. In the present study, a mean overestimation of 2.33 cm d^{-1} (an increase of 89% due to the low flux environment) was found by applying a literature value parameter compared with using the field measurements. Up to a factor of three was found for the most extreme individual cases.

In the study area, the presence of organic matter and changes in sandy lagoon sediments are considered to be the main cause to the variation of thermal conductivities. Similar effects can be observed in other environments because of the usual vegetation growth in the proximities of water bodies shore lines.

The results could be especially relevant for the study of groundwater–surface water interaction trends by explaining discrepancies between flux measurements by different methods, especially in areas with low discharge. Additionally, the measurements of thermal conductivity give the possibility of providing an uncertainty range for the temperature-based estimation of groundwater discharge with a simple methodology and equipment.

Even if the magnitude of changes in flux estimates produced by applying *in situ* measured thermal conductivity is small relative to the flux including this uncertainty range in the flux calculations would help the development of thermal methods used to estimate groundwater discharge to streams, lakes and coastal lagoons.

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