- 1 Thermal conductivity of unfrozen and partially frozen managed peat soils
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Abstract

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Detailed, accurate information on soil temperature is crucial for understanding processes leading to solute leaching and greenhouse gas (GHG) emissions from managed peat soils, but few studies have attempted to study these processes in detail. Drained peat soils have different characteristics from pristine peat. Cultivated peat soils, in particular, have high mineral matter content in the plough layer, due to mineralisation of peat and, sometimes, addition of mineral material. This study examined the effect of mineral matter content on thermal conductivity (λ) in partially frozen and unfrozen peat samples. Effect of change in temperature from -3°C to -10°C on thermal conductivity was also estimated. Three existing models for estimating the thermal conductivity of organic soils were assessed for their suitability for cultivated drained peat soils. The thermal conductivity of peat samples with three different levels of mineral matter content was determined, using the single probe method, in the saturated state and when subjected to at least two different matric potentials at five different temperatures (+10°C, +1°C, -3°C, -5°C and -10°C). The results showed that λ values differed between peat soils depending on mineral matter content, ice content and moisture content. The samples with the highest mineral matter content and bulk density had higher thermal conductivity at positive temperatures and to a lesser extent, at freezing temperatures, when volumetric water content and volume of water-free pores was similar. Most soil samples, especially those with no added mineral soil, were not fully frozen at -3°C and -5°C, but this had minor effect on thermal conductivity compared with values measured at -10°C. The Brovka-Rovdan model proved reasonably good at predicting frozen thermal conductivity in sand-enriched peat soils, while the de Vries model proved best at estimating thermal conductivity for unfrozen peat samples. We provide a first estimate of the thermal conductivity of (partially) frozen cultivated peat measured using undisturbed samples. These

- results can be used to parameterise numerical heat transport models for simulating soil processes
- and GHG emissions.

38 Abbreviations

- 39 VWC = volumetric water content of the soil $(m^3 m^{-3})$
- 40 VWPS = water-filled pore space $(m^3 m^{-3})$
- VAC = volumetric air content of the soil $(m^3 m^{-3})$
- VIC = volumetric ice content of the soil $(m^3 m^{-3})$
- OM = organic matter content (g g^{-1})
- 44 BD = bulk density (g cm $^{-3}$)
- $\lambda = \text{thermal conductivity}$
- von Post scale = degree of humification according to the von Post classification system
- L = peat samples with low mineral matter content,
- M = peat samples with medium mineral content (plough layer of a cultivated peatland site)
- 49 H = manufactured peat samples with high mineral matter content

1. Introduction

Soil thermal conductivity (λ) is a critical parameter controlling soil temperature. It is therefore important to understand variations in thermal conductivity when dealing with temperature regulated soil processes such as decomposition (e.g. Fang and Moncrieff, 2001), nutrient leaching (e.g. Jabloun et al., 2015) and production of greenhouse gases (GHG) (e.g. Schaufler et al., 2010). Land use and management alter peat soil properties, including thermal properties. Drainage increases decomposition rates leading to lower porosity in most peat soils, and cultivation practices further intensify this process (e.g. McLay et al., 1992, Kechavarzi et al., 2010). Moreover, some cultivated peat soils have a high mineral matter content in the plough layer due to deliberate addition of mineral soil as an amendment (Myllys and Soini, 2008). There have been some studies on thermal conductivity in peat samples from pristine mires (e.g. Kettridge and Baird, 2007, Hamamoto et al., 2010, Smerdon and Mendoza, 2010), but not in undisturbed cultivated peat. Moreover, only Konovalov and Roman (1973) and Brovka and Rovdan (1999) have studied the effect of mineral soil inclusion on peat thermal conductivity. There is thus a need for more studies on the effect of changes in peat physical properties on soil thermal conductivity.

In theory, the thermal conductivity of soils is most strongly controlled by the relative fraction of water, ice and air content, as thermal conductivity is much higher for water than for air (de Vries, 1963). Previous studies have found that soil thermal conductivity increases with water content in both mineral and organic soils (e.g. de Vries, 1963). The increase has been found to be almost linear in peat soils (Konovalov and Roman, 1973, Kujala et al., 2008, O'Donnell et al., 2009, Hamamoto et al., 2010, Dissanayaka et al., 2012), although some studies suggest an exponential relationship for peat (Côté and Konrad, 2005). On the other hand, soil thermal conductivity is inversely correlated with air-filled porosity (Ochsner et al., 2001). In addition to water, ice and air content, mineral matter content and organic matter content (OM) are usually

the key factors influencing soil thermal properties, their relative importance depending on circumstances. In organic soils, the thermal conductivity is typically lower than that in mineral soils (especially soils with quartz minerals) and has generally been found to increase with increasing mineral matter content (Brovka and Rovdan, 1999).

Thermal conductivity of water-saturated frozen peat is close to that of ice and higher than that of an unfrozen soil. In general, thermal conductivity does not change significantly with temperature if the soil (peat or mineral) remains either fully unfrozen or fully frozen (e.g. Campbell and Norman, 1998). However, less is known about the thermal conductivity of peat soil that is only partially frozen. Such knowledge is needed as frozen conditions or freezing-thawing processes are important for e.g. estimating GHG production in peatlands. In previous studies on frozen peat soils (Brovka and Rovdan, 1999, Kujala et al., 2008), thermal conductivity has been measured only at a temperatures lower than -10°C, representing totally frozen conditions. Lack of studies at a range of sub-zero temperatures creates problems for accurate modelling of peat soils at negative temperatures close to 0°C, due to the fact that peat only starts to freeze at temperatures lower than -2°C and may not be fully frozen even at -5°C (Konovalov and Roman, 1973, Smerdon and Mendoza, 2010).

In this study, thermal conductivity was examined at five different temperatures (T) ranging from +10°C to -10°C including partly frozen conditions (T = -3°C and -5°C) in a laboratory setting. Furthermore, samples with differing mineral matter content representing different cultivated peat soils, and subjected to different soil matric potentials, representing different water drainage depths, were tested. The research questions were: I) Does high mineral matter content, often observed for cultivated peat soil, result in substantially different thermal conductivity compared to other drained peat soil? II) Does the ice content in peat increase with decreasing temperature from -3°C to -10°C so much that the thermal conductivity substantially increases? III) Which of the three empirical thermal conductivity models tested is best for

- estimating the thermal conductivity of peat soils with different mineral matter contents (in frozen
- and unfrozen state)?

2. Materials and methods

1.1 Study sites

The samples used in this study were boreal fen peat collected from the partly drained Pelso peatland complex in Northern Finland, which comprises a cultivated peatland area, a peatland forest and a peat extraction site (see Mustamo et al., 2016 for detailed description). The thermal conductivity models were also tested with undisturbed samples from two depths (10-20 cm and 30-40 cm) of two cultivated peatland sites, Majnegården and Örke, in Sweden (see Berglund and Berglund, 2011 for further details of these sites.) These additional samples were included to increase the generalisability of the model test results by adding variety to physical properties of the samples (while keeping manipulation of samples to a minimum).

The cultivated peat at Pelso was first drained in the 1930s and since then the field has been under a rotation with timothy grass (*Phleum pratense*) for 3-4 years, followed by one year of barley (*Hordeum vulgare*). Mineral soil and lime have been mixed into the topsoil of the peat (mainly *Carex* peat) since initial drainage, to enhance the cultivation properties. Chemical fertiliser has also been regularly applied at the site. Mean groundwater depth during the growing season of 2012 was 40-65 cm below peat surface, depending on the location of measurement. The forest site is inefficiently drained (mean groundwater depth during the growing season of 2012 was 16-22 cm below soil surface), resulting in ponding water in some places. Partly for this reason, the forest is a poorly growing dwarf shrub-type forest that has not been fertilised or limed since drainage in the 1970s. The main peat type is *Carex* at the forest site. The peat extraction site was a former peatland forest (similar to that described above), which was drained in 2006 and the uppermost peat layer removed. The remaining peat is mostly *Carex* mixed with *Sphagnum* peat at this site. Mean groundwater depth during the growing season of 2012 was 67 cm below peat surface at the peat extraction site.

The Majnegården site has been used for grass and silage production and cattle grazing since drainage in the 1920s (Kasimir Klemedtsson et al., 2009), whereas Örke was drained in 1938 and is now under permanent pasture (McAfee, 1985). The Majnegården site has a layered structure with a highly decomposed plough layer down to about 25 cm depth (with mineral material and shells) and poorly decomposed soil below that, the peat being mainly reed peat (Berglund and Berglund, 2011). The peat at the Örke site is mainly a sedge-brown moss peat and is highly decomposed, but with low mineral matter content (Berglund and Berglund, 2011). The porosity of the topsoil at Majnegården is lower than at Örke, but soil water content at 40 cm and 80 cm drainage depth is similar in both soils, which results in a higher proportion of air-filled pores in the profile at Örke at these drainage depths (Berglund and Berglund, 2011).

1.2 Soil samples

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Undisturbed and disturbed (manufactured) peat samples were collected from the Pelso study sites. The undisturbed, moderately decomposed (approximately H4-H6 on von Post scale) samples were taken in sharpened PVC pipes (volume 1100 cm³, inner diameter 10 cm, height 12-13 cm). Eight samples were taken from the peat extraction site (4 samples from 2-15 cm depth, 4 samples from 42-55 cm depth) and eight from the peatland forest (from 2-28 cm depth after removal of vegetation and an undecomposed moss layer), where the soil was pure peat with no added mineral matter. These samples had low mineral matter content (L samples). Sixteen undisturbed peat samples were also taken from the plough layer (2-15 cm) of the cultivated *Carex* peat site and these samples had medium mineral matter content (M samples). To increase the range of organic matter contents, an additional 16 samples were manufactured by mixing peat from the peat extraction site (from depth 0-70 cm) at its water content with mineral soil (particle size <2 mm, particle density 2.7 g cm⁻³) using a peat:mineral soil mass ratio of 1:0.6. The samples were compacted by hand. These samples had high mineral matter content (H samples). All 48 samples of Pelso peat were drained to different water contents by a pressure plate device (e.g. Laurén and Heiskanen, 1997, Ronkanen and Kløve, 2005), with the pressure maintained for at least 7 days. After that time, a few drops of water were still leaving the samples but most of the water extractable by this method had been removed. Therefore, the water content reached was considered a close enough approximation of the true equilibrium water content corresponding to the matric potential in question. Four different moisture levels were created: fully saturated samples and samples with water content corresponding approximately to matric potential of -10 kPa, -40 kPa (only for L and M samples) and -500 kPa, which correspond to -100 cm, -400 cm and -5000 cm of water column, respectively. The final volumetric water content (VWC) range at saturated, -10 kPa, -40 kPa and -500 kPa matric potential was 0.67-0.90, 0.57-0.86, 0.62-0.76 and 0.46-0.72 m³ m⁻³, respectively. Drainage in the pressure chamber caused the samples to shrink (median 10%, max. 18%), although the H samples shrank considerably only

at -500 kPa matric potential. For M samples, shrinkage at -10 kPa level was not measured. Shrinkage of samples was accounted for in the calculations by taking the reduced sample volume as total volume of the sample and assuming that the reduction was due to a decrease in pore volume. When the samples were frozen at -10°C, about 10-20% of the water was still unfrozen. However, there is some uncertainty associated with this estimate, which is based on the difference in VWC measured in the frozen state (using sensors) and the unfrozen state (calculated from oven drying), due to sensor error and the fact that the value calculated from oven drying was for the whole samples, whereas the sensors did not reach the lowest part of the samples. Despite this uncertainty, the peat samples could not be assumed to be fully frozen at temperatures close to 0°C. Undisturbed samples from the 10-20 cm and 30-40 cm soil horizons at Majnegården and Örke were drained using the sand box method (Andersson, 1955), to a water content equivalent to drainage depth of 0.05 m, 0.4 m and 0.8 m (equivalent to -0.5, -4 and -8 kPa). When estimating thermal conductivity for these samples using models, porosity and VWC values estimated for each site and soil horizon based on Berglund et al. (2010) were used (Table 1). For the samples representing drainage of 0.05 m, VWC was calculated from porosity by assuming a water-filled pore space (WFPS) of 98%. Mass of solids (m_{solids}) was calculated as product of BD and sample volume. Mass of mineral matter fraction $(m_{\rm m})$ was calculated as product of mineral matter content (1-OM) and m_{solids} . The volume of mineral matter fraction was calculated as product of

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Table 1. Soil porosity, volumetric water content (VWC) and water-filled pore space (WFPS) in samples from the 10-20 cm and 30-40 cm soil layers at the Majnegården and Örke sites, estimated based on Berglund et al. (2010) and additional material.

Majnegården	Örke
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 $m_{\rm m}$ and estimated particle density for mineral soil (2.7 g/cm³ (de Vries, 1963)).

soil depth (cm)	drainage treatment group (m)	Porosity (m ³ m ⁻³)	VWC (m ³ m ⁻³)	WFPS (m ³ m ⁻³)	Porosity (m³ m-³)	VWC ($m^3 m^{-3}$)	WFPS (m ³ m ⁻³)
10-20	0.05	0.69	0.68	0.98	0.81	0.79	0.98
	0.4	0.69	0.63	0.91	0.81	0.69	0.85
	0.8	0.69	0.60	0.87	0.81	0.66	0.82
30-40	0.05	0.88	0.87	0.98	0.86	0.84	0.98
	0.4	0.88	0.85	0.96	0.86	0.76	0.89
	0.8	0.88	0.82	0.93	0.86	0.73	0.85

1.3 Measurement of thermal conductivity

The undisturbed and disturbed samples from Pelso were wrapped tightly in three layers of plastic sheeting, fitted into water-tight plastic containers and placed in a a LAUDA RK 20 KS Compact Low-Temperature Thermostat chamber (filled with circulating antifreeze liquid) to reach the desired temperature. Thermal conductivity was measured at +1°C, -3°C, -5°C and -10°C and, for the L samples and M samples, also at +10°C. Each measurement was performed on four replicate samples, but in some cases results from only 2-4 samples were included in the analysis, due to indications of measurement errors (such as probe malfunction). To eliminate an initially observed vertical temperature gradient in the samples, the samples (other than M samples in saturated state and at -10 kPa and -40 kPa matric potential) were covered with additional insulating material before temperature measurement. However, the problem was not entirely removed, as a temperature difference of 1.5°C was observed between the top of the sample and 9 cm depth. Thermal conductivity was measured using the single probe method (Farouki, 1986, Laurén, 1999), with probe length 7.5-10 cm (diameter 3 mm), heating time 15 min, resistor wire

resistance 11.5-33.7 ohms and current 0.04-0.15 mA (Fig. 1). The temperature change was kept as less than 2°C by adjusting the current to prevent the melting. We did observe regions of slower increase of temperature in response to heating in temperature curves (which would have indicated melting) in some measurement, and these measurements were excluded. The mean of 2-3 successful measurements was used as the final λ value for each sample at the given water content. During the measuring sequence, soil temperature was monitored with a K-type wire connected to a Beamex Precision Thermometer TC-301, while VWC was measured with a Decagon EC-H2O Soil Moisture Sensor EC-5 probe calibrated for this type of peat soil. Soil VWC was also determined by drying the samples at 65°C (this temperature was chosen to avoid charring and the sample mass was carefully monitored until it stopped decreasing). OM was determined by incineration at 550°C (two replicates). Volumetric ice content was calculated as the difference in VWC measured in the frozen state (using Soil Moisture Sensor) and the unfrozen state (calculated from oven drying). The thermal conductivity of the samples from Majnegården and Örke was measured at +20°C and -11°C (mean of 1-2 replicate measurements per sample, 1-3 samples per soil horizon/drainage level/temperature combination), using similar methods as for the Pelso samples, except that the temperature of -11°C was achieved using a freezer.

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1.4 Models for estimating thermal conductivity

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Three well-known empirical models for determining the thermal conductivity of unfrozen peat were tested using the measured data from peat samples collected in this study. These were the de Vries (1963) model, the Dissanayaka et al. (2012) model and the Brovka and Rovdan (1999) model. The constants used in this study are presented in Table 2.

- Model 1: The classic empirical model for calculating the thermal conductivity of organic soil
- developed by de Vries (1963) (valid for volumetric air content VAC <0.50 m³ m⁻³):

$$\lambda = (\theta \cdot \lambda_{water} + k_o \cdot \sigma_o \cdot \lambda_o + k_m \cdot \sigma_m \cdot \lambda_m + k_a \cdot \epsilon \cdot \lambda_{app}) / (\theta + k_o \cdot \sigma_o + k_m \cdot \sigma_m + k_a \cdot \epsilon)$$
 (1)

where

- θ = water fraction (m³ m⁻³)
- σ_0 = organic matter fraction (m³ m⁻³)
- $\sigma_{\rm m}$ = mineral soil fraction (m³ m⁻³)
- $\varepsilon = \text{air fraction (m}^3 \text{ m}^{-3})$
- k_o = organic phase weight factor calculated with Eq. 2
- k_m = mineral soil phase weight factor calculated with Eq. 3
- k_a = air phase weight factor calculated with Eq. 4

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$$k_0 = \frac{1}{3} \sum_{i=a,b,c} \left[1 + \left[\frac{\lambda_0}{\lambda_{\text{water}}} - 1 \right] gi \right]^{-1}$$
 (2)

$$k_{\rm m} = \frac{1}{3} \sum_{i=a,b,c} \left[1 + \left[\frac{\lambda \rm m}{\lambda \rm water} - 1 \right] g i \right]^{-1}$$
 (3)

$$k_{a} = \frac{1}{3} \sum_{i=a,b,c} \left[1 + \left[\frac{\lambda app}{\lambda water} - 1 \right] g_{i} \right]^{-1}$$

$$(4)$$

Model 2: An empirical model for estimating λ of peat by Dissanayaka et al. (2012) (Eq. 5).

$$\lambda = 0.225 \cdot \sigma + 0.025 + 0.89 \cdot \lambda_{\text{water}} \cdot \theta$$
 (5)

where σ = fraction of soil solids (m³ m⁻³).

- 251 Model 3: An empirical model developed by Brovka and Rovdan (1999), which is valid for peat-
- sand mixtures with less than 0.96 % by weight of sand.

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 $\lambda = a_0 + a_1 \cdot x_{water} + a_2 \cdot x_{sand} \cdot x_{peat} + a_3 \cdot x_{sand} \cdot x_{water} + a_4 \cdot x_{sand}^2 + a_5 \cdot x_{peat}^2 + a_6 \cdot x_{water}^2$ (6)

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- where
- $x_{\text{water}} = \%$ (by weight) of water in unfrozen sample
- $x_{sand} = \%$ (by weight) of sand in unfrozen sample
- $x_{peat} = \%$ (by weight) of peat in unfrozen sample.

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- In the present study, this model was tested both for unfrozen and frozen samples. The % (by
- weight) of sand (x_{sand}) was approximated to equal sample ash content.

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Table 2. Parameters used in the de Vries model (Eqs. 1-4) and model constant values given by de Vries (1963) and Brovka & Brovdan (1999) b.

Symbol	Constants	Value	Note
$\lambda_{\mathrm{water}}^{}a}$	Thermal conductivity of water	$0.57~{\rm W}~{\rm m}^{-1}~{\rm K}^{-1}$	
λ_{o}^{a}	Thermal conductivity of organic matter	$0.25~{\rm W}~{\rm m}^{-1}~{\rm K}^{-1}$	
λ_m^{a}	Thermal conductivity of mineral soil	$^{\circ}$ 2.9 W m ⁻¹ K ⁻¹ 8.8 W m ⁻¹ K ⁻¹	for clay for quartz
$\lambda_{app}{}^a$	Apparent thermal conductivity of gas-filled pore space	$0.05~{ m W}~{ m m}^{-1}~{ m K}^{-1}$	for air with water vapour
$g_a{}^a$	Particle shape factor	0.5	assumes cylindrical soil particle shape
g_b^a	Particle shape factor	0.5	assumes cylindrical soil particle shape
g_c^a	Particle shape factor	0	assumes cylindrical soil particle shape
a_0^b	Empirical constant	$1.98 \cdot 10^{-2} $ $2.38 \cdot 10^{-2}$	unfrozen soil frozen soil
a_1^b	Empirical constant	$6.56 \cdot 10^{-4} \\ 5.37 \cdot 10^{-4}$	unfrozen soil frozen soil
a_2^b	Empirical constant	$-1.22 \cdot 10^{-6}$ $-3.47 \cdot 10^{-6}$	unfrozen soil frozen soil
a_3^b	Empirical constant	$8.69 \cdot 10^{-7} \\ 2.75 \cdot 10^{-6}$	unfrozen soil frozen soil
a_4^b	Empirical constant	$6.43 \cdot 10^{-7} \\ 8.81 \cdot 10^{-7}$	unfrozen soil frozen soil
a_5^b	Empirical constant	$2.11 \cdot 10^{-7} $ $2.04 \cdot 10^{-7}$	unfrozen soil frozen soil
a_6^b	Empirical constant	$-1.24 \cdot 10^{-7}$ $1.71 \cdot 10^{-6}$	unfrozen soil frozen soil

1.5 Analysis of thermal conductivity data

All data analysis was performed with R-software (version 3.4.2). The statistical testing was performed using a mixed model (lme-function from nlme-package; Pinheiro et al., 2017), with individual sample (sample_id) as random effect (random intercept) using Restricted Maximum Likelihood (REML). Analysis was performed separately for the frozen and unfrozen samples. The thermal conductivity was log-transformed, based on model diagnostics suggesting non-normality of residuals and heteroscedasticity of residual variances without transformation.

Overall significance of variable effects was determined by comparing models with and without variable effects. Comparison of models was based on likelihood ratios (by setting up alternative models using maximum likelihood instead of REML and then using the anova.lme command).

The individual models used in data analysis are shown in Appendix A.

The performance of thermal conductivity models by de Vries (1963) and Brovka and Brovdan (1999) and Dissanayaka et al. (2012) was compared using Lin's (1989, 2000) concordance correlation coefficient (CCC) (epiR-package; Nunes et al., 2018).

2 Results and Discussion

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2.1 Observed physical characteristics of the peat samples

Physical properties of the peat depended on sampling site: samples from the plough layer of the Pelso cultivated site differed clearly from the non-cultivated peat samples. This was expected, since cultivation changes the porosity and bulk density (BD) of the plough layer. The main reasons are that peat is compacted due to the effect of mineralisation, physical ploughing and addition of mineral soil (Kechavarzi et al., 2010, McLay et al., 1992, Myllys and Soini, 2008). The L samples (pure peat) had the highest organic matter (lowest mineral matter) content (median OM content 0.97 g g⁻¹) (Table 3). The M samples (from the plough layer of the cultivated peat site) had clearly lower median OM content (median 0.56 g g⁻¹) due to cultivation practices, while the H samples (manufactured peat-sand mixture) had the lowest OM content (median 0.17 g g⁻¹). However, estimated OM content was quite similar for all three groups of samples (Fig. 2). The L samples had the highest porosity and lowest BD, while the H samples had the lowest porosity and highest BD (Table 3). The organic matter content of the M samples were similar to that in both soil layers of the Majnegården peat (Table 3). The soil at Örke is highly decomposed but has a low mineral soil content, and thus more resembled L samples. As expected, VWC decreased with increasing matric potential. The H samples (manufactured peat-sand mixture) were drier than the M and L samples when saturated or at -10 kPa matric potential, but VWC was more similar across sample groups at -500 kPa (Fig. 2, Fig. 3).

Table 3. Median values (min-max) of soil properties of Pelso samples with high (H), medium (M) and low (L) mineral matter content and of the 0-20 cm and 30-40 cm soil horizons at Majnegården and Örke (Berglund and Berglund, 2011). n = number of replicate samples

Soil sample	. •	n	Organic	n	Bulk density	n	Degree of
group	$(m m^{-3})$		matter				decomposition
			content		(~ ~~-3)		(111 1110
			$(g g^{-1})$		$(g cm^{-3})$		(H1–H10
			C1 f-	D	-1		von Post scale)
-			Samples fr				
L	0.86	4	0.97	16	0.18	4	H46
	(0.84-0.90)		(0.93-0.98)		(0.14-0.22)		
M	0.77	3	0.56	19	0.34	3	H4
	(0.74-0.80)		(0.23-0.66)		(0.33-0.37)		
Н	0.67	3	0.17	10	0.62	3	na
	(0.67-0.68)		(0.11-0.31)		(0.60-0.65)		
		S	amples from	Majn	egården site		
0-10 cm	0.69	4	0.64	16	0.64	4	H7–8
	(0.68-0.71)		(0.62 - 0.64)		(0.60-0.66)		
30–40 cm	0.88	4	0.76	8	0.21	4	H1–2
	(0.88-0.89)		(0.75-0.80)		(0.19-0.22)		
	•		Samples f	rom Ö	Orke site		
5-15 cm	0.81	4	0.86	34	0.31	4	H9–10
	(0.80 - 0.82)		(0.84-0.86)		(0.28-0.33)		
30–40 cm	0.86	4	0.87	34	0.23	4	H8–9
	(0.85 - 0.87)		(0.84-0.89)		(0.21-0.23)		

na = data not available. Note that OM values for the Pelso samples include all values determined for these samples, including samples for which thermal conductivity readings were discarded.

2.2 Observed thermal conductivities

Peat decomposition or sand addition to the topsoil layer increases the mineral matter content of the peat. Higher mineral matter content was expected to result in higher thermal conductivity (Konovalov and Roman, 1973, Brovka and Rovdan, 1999). The highest λ values for unfrozen samples (median 0.85 W m⁻¹ K⁻¹) were indeed found for the H samples with the highest mineral matter content. However, the unfrozen thermal conductivity of the undisturbed M and L samples did not differ substantially (median 0.58 W m⁻¹ K⁻¹ and 0.52 W m⁻¹ K⁻¹, respectively) (Table 4). The undisturbed samples of cultivated peat from Majnegården and Örke had the lowest unfrozen λ values. Overall, the measured λ values were similar to literature values reported for peat, which

are generally within the range 0.2-0.8 W m⁻¹ K⁻¹ (Brovka and Rovdan, 1999, Kettridge and Baird, 2007, Kujala et al., 2008, Hamamoto et al., 2010).

The λ values obtained for frozen samples had high variation but had median values of 1.5 W m⁻¹ K⁻¹, 1.5 W m⁻¹ K⁻¹ and 1.2 W m⁻¹ K⁻¹ for the H samples, M samples and L samples, respectively. In frozen state, the Majnegården and Örke samples showed λ values of 0.84-1.4 W m⁻¹ K⁻¹ (Table 5). The maximum observed values were somewhat higher than those reported in previous studies, which have generally been within the range 0.2-2.0 W m⁻¹ K⁻¹ (Konovalov and Roman, 1973, Brovka and Rovdan, 1999, Kujala et al., 2008), depending on mineral matter content and water content. This is likely because the VWC of the samples in this study was quite high, so the ice content of the frozen samples was also high (note that λ_{ice} is 2.2 W m⁻¹ K⁻¹, λ_{water} is 0.567 W m⁻¹ K⁻¹ and λ_{air} is 0.024 W m⁻¹ K⁻¹).

Table 4. Median thermal conductivity (W m⁻¹ K⁻¹, minimum and maximum in brackets) at different matric potential values of unfrozen (T = +1°C) and frozen (T = -10°C) Pelso peat samples with high (H), medium (M) and low (L) mineral content. n = number of replicate samples.

samples.						
measurement						334
conditions	L	n	M	n	Н	n
	Unfroz	zen	condition at T	$\vec{r} = +$	·1°C	335
Saturated	0.54	4	0.66	3	0.92	3363
	(0.50-0.60)		(0.63-0.74)		(0.88-1.4) 337
-10 kPa	0.50	4	0.61	3	0.87	4
	(0.34-0.60)		(0.52-0.64)		(0.79-1.0	338
-40 kPa	0.49	4	0.42	3	na	,
	(0.30-0.58)		(0.38-0.49)			339
-500 kPa	0.38	4	0.52	4	0.61	3403
	(0.22-0.54)		(0.49-0.55)		(0.56-0.62)	2)
	Fully fr	oze	n condition at	T=	-10°C	341
Saturated	1.7	4	2.3	3	2.3	3423
	(1.6-2.2)		(1.6-2.4)		(2.0-2.4)	343
-10 kPa	1.5	4	1.6	3	1.5	4
	(0.68-1.6)		(1.2-1.9)		(1.3-1.7)	344
-40 kPa	1.2	4	0.50	3	na	
	(0.64-1.5)		(0.35-0.66)			345
-500 kPa	0.49	4	1.1	4	1.0	3463
	(0.33-1.1)		(0.80-1.2)		(0.67-1.1	
	,		, , , , ,		•	347

Table 5. Thermal conductivity (λ, W m⁻¹ K⁻¹) of peat samples from Majnegården and Örke at different soil horizon, temperature and drainage levels. Values shown are mean of 1-3 samples at each soil horizon/temperature/drainage level. Drainage depth of 0.05 m, 0.4 m and 0.8 m are equivalent to -0.5, -4 and -8 kPa.

Drainage depth (m)	e Majnegårder	n	Örke	
	10-20 cm	30-40 cm	10-20	30-40
			cm	cm
	λ(Wr	m ⁻¹ K ⁻¹) at +	20°C	
0.05	0.53	0.49	0.48	0.48
0.4	0.50	0.49	0.43	0.45
0.8	0.51	0.54	0.42	0.45
	λ (W 1	m ⁻¹ K ⁻¹) at -1	1°C	
0.05	1.2	1.4	1.1	1.1
0.4	1.1	1.1	0.84	0.89
0.8	1.0	1.3	0.84	0.88

2.3 Effect of soil characteristics on thermal conductivity

2.3.1 Drainage level did not fully explain the differences in observed thermal conductivities

The M and H samples had significantly higher unfrozen and frozen thermal conductivity than the L samples when temperature and matric potential treatment (representing drainage depth) were taken into account in the analysis (Appendix B). The sample group (L, M or H) was very significant in estimating unfrozen λ (likelihood ratio: 35.3, p<0.0001), but also in estimating frozen λ (likelihood ratio: 16.9, p=0.0098). The difference in frozen λ between M and H samples was very small, whereas the unfrozen λ of H samples was considerably higher than that of M samples (Appendix B). It should be noted that the difference between the M and L groups almost disappeared when the samples with -40 kPa matric potential treatment were included in the comparison (there was no data on group H for the -40 kPa matric potential treatment). This seems to be due to the M samples in this treatment having had unusually low thermal conductivity. The results indicate that the plough layer of cultivated peat soils should be considered as a separate layer when thermal content is used as parameter in physical models that use groundwater depth to estimate soil water content. However, under field conditions, plant water uptake, specific soil cover and weather conditions also regulate soil water content, in addition to groundwater depth, so these results cannot be directly applied in models that do not consider those factors.

2.3.2 Group H samples had higher thermal conductivity after accounting for VWC, VAC and VIC

The H samples were found to have higher unfrozen λ than the M and L samples, which had similar values, after accounting for VWC, VAC and VIC (Appendix B, Fig. 4). The effect of VWC, VAC and VIC had to be excluded when estimating the effect of mineral matter content, as thermal conductivity correlated with VAC (Pearson correlation coefficient r=-0.54) and, for

the frozen samples, with VIC (r=0.34). These two variables were also correlated with each other (r=-0.57), so distinguishing their individual effects was not possible. Within peat sample groups (L, M, H), there was also a correlation between λ and VWC (r = 0.57 to 0.77).

Sample group was significant in estimating unfrozen λ with VAC and VWC included in the model (likelihood ratio: 17.9, p<0.0001), but the sample group only had a weak significance for frozen λ (likelihood ratio: 6.9, p-value: 0.032). These findings agree with Brovka and Rovdan (1999), who showed that in unfrozen peat λ increases with sand content, but that in frozen samples the effect depends on soil water content. However, in the present study, M samples had somewhat lower frozen and unfrozen λ than L samples after accounting for VWC, VAC and VIC (Appendix B). This may be due to the anomaly that the M samples which were treated at matric potential -40 kPa had very low λ values. The soil properties of this sub-group of M samples did not explain their low λ values. If the M samples at matric potential -40 kPa were excluded from the analysis, the M samples had somewhat higher λ than the L samples (Appendix B), the significance of sample group to model also decreasing slightly (likelihood ratio: 13.4, p=0.0012). The differences in porosity ranges observed in each sample group (H, M and L) introduce uncertainty to results as there is no data on λ for all combinations of VWC and VAC for each sample group. A study with more samples from different cultivated peat soils would increase the reliability of this result.

According to the model without the samples at -40 kPa, at average VWC and VAC the difference in unfrozen λ between H and L samples was around 0.2 W m⁻¹ K⁻¹, whereas difference in unfrozen λ between M and L samples was only around 0.02 W m⁻¹ K⁻¹. Similarly, the difference in frozen λ between H and L samples was around 0.3 W m⁻¹ K⁻¹, while between M and L samples it was only around 0.07 W m⁻¹ K⁻¹. Thus, it appears that when data are available on actual VWC

and porosity, the plough layer of cultivated peat soils should be considered as a separate layer in physical models only for the most mineral-soil enriched sites, while for most management planning purposes this is likely unnecessary.

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2.4 Ice content and frozen thermal conductivity increased slightly with decreased temperature

There was a statistically significant difference between frozen λ at -3°C, -5°C and -10°C when sample group, unfrozen sample VAC and unfrozen sample VWC were also accounted for (likelihood ratio: 9.4, p=0.0092). However, the actual observed increase in λ from -3°C to -10°C was not very large. For instance, for L samples with average unfrozen VAC and VWC, the increase was approximately from 1.15 W m⁻¹ K⁻¹ to 1.21 W m⁻¹ K⁻¹ (Appendix B). This change is likely due to increased ice content, e.g. the ice content in the average L sample would have increased approximately from 0.45 to 0.49 m³ m⁻³ (Appendix B). It appears that soil temperature difference between -3°C and -10°C does not need to be taken into account when estimating thermal conductivity of peat. However, it is important to consider that this observation only holds for temperatures lower than -3°C, and in some peatland regions, e.g. in southern Sweden and southern Finland, the most common wintertime temperature even in topsoil may exceed -3°C. For example, in a lysimeter study with undisturbed peat soil from Majnegården and Örke conducted at Ultuna in southern Sweden (Berglund and Berglund, 2011), soil temperature mainly stayed close to 0°C during the winter, indicating partial freezing in the topsoil (unpublished data). In that study, a decrease in VWC at 20 cm was observed only at the end of March and soil temperature at 20 cm depth did not drop below -3°C at any point during the winter. In those conditions, the unfrozen water content of peat reached about 0.40-0.50 m³ m⁻³ in the field (in comparison, the unfrozen water content of the frozen Pelso samples at -10°C was lower, 0.10-0.20 m³ m⁻³). For a region such as Ultuna the effect of sub-zero temperature on thermal conductivity is likely stronger than observed in this study and should not be ignored.

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2.5 De Vries model was best for estimating unfrozen thermal conductivity

The mineral soil content of the samples affected the fit of the unfrozen peat λ models tested (Fig. 5). All three models showed relatively good fit for samples with low mineral soil content (Table 6). The classic de Vries model was the best predictor of λ for the L and M samples, while the Brovka-Rovdan model and especially the Dissanayaka et al. model underestimated λ for these samples (Fig. 5). The fit of the de Vries model for H samples was the best when the thermal conductivity of the mineral fraction (\(\lambda_m\)) was assumed to be between the values for quartz sand and clay (Fig. 5). This also agrees with findings by Konovalov and Roman (1973) of different thermal conductivity in sandy peats than clayey peats. For the undisturbed samples in the present study (M samples and Majnegården plough layer samples), the fit of the de Vries model was much better with the lowest λ_m value tested (2.9 W m⁻¹ K⁻¹, for clay). It appears that mineral matter type, if known, should be considered when using the de Vries model to estimate thermal conductivity for the plough layer of cultivated peat soils, especially when the mineral matter content is over 40 m-%, as observed in the disturbed samples in this study. The Dissanayaka et al. model, originally developed for pure peat samples, was the most sensitive to sand content in the soil and did not give a good fit to observations for M or H samples (Fig. 5, Table 6). The Brovka-Rovdan model, which assumes fully frozen soil, gave a reasonably good fit for all frozen samples (CCC = 0.58), although it had a tendency to overestimate the thermal conductivity of samples at lower soil water content (Fig. 6). The fit of the model was not markedly different across sub-zero temperatures. This indicates that while the ice content still changed as the temperature decreased from -3°C to -10°C, especially for the saturated samples with low mineral matter content, this did not affect soil thermal conductivity in a significant way.

Table 6. Model fit (Concordance Correlation Coefficient) of the de Vries, Brovka & Rovdan and Dissanayaka et al. models in estimating the thermal conductivity of Pelso peat soils with high (H), medium (M) and low (L) mineral matter content and of Örke and Majnegården peat soil layers. λ_m = thermal conductivity of mineral matter

Model	All samples	Low mineral matter content (L samples, Örke samples and Majnegården samples of 30-40 cm depth)	Medium mineral matter content (M samples, Majnegården samples of 10-20 cm depth)	High mineral mater content (H samples)
De Vries, λ_{m} = 5.6 W m ⁻¹ K ⁻¹	0.81	0.67	0.38	0.32
De Vries, $\lambda_{m}=2.9 \text{ W m}^{-1} \text{ K}^{-1}$	0.70	0.67	0.38	0.22
De Vries λ_{m} = 8.8 W m ⁻¹ K ⁻¹	0.71	0.67	0.17	0.15
Brovka & Rovdan, unfrozen samples	0.69	0.60	0.33	0.24
Brovka & Rovdan, frozen samples	0.58	0.59	0.46	0.51
Dissanayaka et al.	0.08	0.58	0.14	0.04

3 Conclusions

- Peat soil samples with the highest proportion of mineral matter had the highest thermal conductivity in unfrozen condition. The samples with the highest mineral soil content had the highest thermal conductivity even when considering volumetric air and water content. However, it seems that in most cases, this only needs to be considered when modelling cultivated peat soil with higher mineral matter content than the cultivated site sampled in this study. This study differed from most previous studies on thermal conductivity of peat by using undisturbed samples, but a wider study on thermal regimes of cultivated peat soil in field conditions would bring even more insight on the practical significance of the observed differences.
- Peat soil samples, especially pure peat, were not fully frozen at -3°C and -5°C, but this did not have a considerable effect on λ compared with that at -10°C. However, this result does not necessarily apply for temperatures between -3°C and 0°C. A study with different methodology is needed to establish how thermal conductivity of peat changes in that critical temperature range.
- The best model for predicting the thermal conductivity of unfrozen mineral soil-enriched
 peat was found to be the classic de Vries model. The Brovka-Rovdan model also
 performed reasonably well for frozen peat soils and for unfrozen peat soils with low
 mineral matter content.

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Appendix A. R syntax of models used in the analysis

573

```
The effect of sample group (sample group) on thermal conductivity at different temperature
574
      (temperature group, levels: unfrozen, -3°C, -5°C, -10°C) and matric potentials
575
576
      (matric potential, levels: saturated, -10 kPa, -500 kPa) was examined with model m1.
577
      The full models were m1.unfrozen.a and m1.frozen.a:
578
      m1.unfrozen.a <- lme(log(thermal conductivity)) ~ matric potential* sample group,
579
      random = \sim 1|sample id, ...,
580
      method = "REML")
581
582
      m1.frozen.a <- lme(log(thermal conductivity)) ~ temperature group*matric potential*
583
      sample group,
584
      random = \sim 1|sample id, ...,
585
      method = "REML")
586
587
      The final models with significant effects were m1.unfrozen.b and m1.frozen.b:
588
      m1.unfrozen.b <- lme(log(thermal conductivity)) ~ matric potential + sample group,
589
      random = \sim 1|sample id, ...,
590
      method = "REML")
591
592
      m1.frozen.b <- lme(log(thermal conductivity)) ~ matric potential + sample group,
593
      random = \sim 1|sample id, ...,
594
595
      method = "REML")
```

```
The effect of sample group on thermal conductivity when standardized in respect to (centred)
```

- volumetric percentage of air (VAC), water (VWC) and ice (VIC; only for frozen samples) was
- examined with model m2.
- The **full models** were m2.unfrozen.a and m2.frozen.a :

```
601
```

- 602 m2.unfrozen.a <- lme(log(thermal_conductivity)) ~ VAC*VWC + sample_group,
- for random = $\sim 1 | \text{sample_id}, \dots,$
- 604 method = "REML")

- 607 + VIC:VWC + sample group,
- for random = ~ 1 sample id, ...,
- 609 method = "REML")

610

The **final models** with significant effects were m2.unfrozen.b and m2.frozen.b:

612

- 613 m2.unfrozen.b <- lme(log(thermal conductivity)) ~ VAC+ VWC + sample group,
- for random = ~ 1 | sample id, ...,
- 615 method = "REML")

616

- 617 m2.frozen.b <- lme(log(thermal conductivity)) ~ VAC+ VWC + VIC + VAC:VIC +
- sample group,
- random = ~ 1 | sample id, ...,
- 620 method = "REML")

- The effect of temperature on the thermal conductivity of frozen samples was examined with
- model m3.

- $625 \qquad m3 <- lme(log(thermal_conductivity)) \sim unfrozen_VAC + unfrozen_VWC + sample_group,$
- for random = $\sim 1 | \text{sample_id}, \dots,$
- method = "REML")

628

The effect of temperature on ice content was examined with model m4.

630

- 631 m4 <- lme(VIC ~ unfrozen VAC+ unfrozen VWC + sample group,
- random = $\sim 1 | \text{sample_id}, \dots,$
- 633 method = "REML")

Appendix B. Model summary tables

The models are defined in Appendix A. SE = Standard Error, df= degree of freedom

Model m1.unfrozen.b

	Value	SE	df	<i>t</i> -value	<i>p</i> -value
(Intercept)	-0.738	0.0663	125	-11.1	< 0.001
matric_potential-500kPa	-0.213	0.075	27	-2.84	0.00839
matric_potentialSaturated	0.143	0.0769	27	1.86	0.0737
sample_groupHigh	0.556	0.0762	27	7.29	< 0.001
sample_groupMedium	0.277	0.0741	27	3.74	< 0.001

Model m1.frozen.b

	Value	SE	df	<i>t</i> -value	<i>p</i> -value
(Intercept)	0.1	0.0999	249	1	0.317
matric_potential-500kPa	-0.606	0.112	27	-5.4	< 0.001
matric_potentialSaturated	0.314	0.115	27	2.73	0.0109
sample_groupHigh	0.343	0.112	27	3.05	0.00513
sample_groupMedium	0.338	0.112	27	3.01	0.00565

642 Model m2.unfrozen.b

	Value	SE	df	<i>t</i> -value	<i>p</i> -value
(Intercept)	-0.653	0.0814	160	-8.03	< 0.001
VWC_centred	-0.0101	0.01	34	-1.01	0.321
VAC_centred	-0.0289	0.0102	34	-2.83	0.00769
sample_groupHigh	0.321	0.196	34	1.64	0.11
sample_groupMedium	-0.0231	0.134	34	-0.173	0.864

Model m2.unfrozen.b, without samples in matric potential treatment group -40 kPa

	Value	SE	df	<i>t</i> -value	<i>p</i> -value
(Intercept)	-0.639	0.0856	125	-7.46	< 0.001
VWC_centred	-0.0107	0.00976	27	-1.09	0.284
VAC_centred	-0.0289	0.0102	27	-2.82	0.00898
sample_groupHigh	0.339	0.188	27	1.8	0.0824
sample_groupMedium	0.035	0.134	27	0.262	0.796

647 Model m2.frozen.b

	Value	SE	df	<i>t</i> -value	<i>p</i> -value
(Intercept)	0.146	0.193	299	0.757	0.45
VWC_centred	-0.0214	0.0214	299	-0.999	0.319
VAC_centred	-0.0581	0.0213	299	-2.73	0.00666
VIC_centred	-0.00863	0.0206	299	-0.419	0.676
sample_groupHigh	0.076	0.392	36	0.194	0.847
sample_groupMedium	-0.229	0.267	36	-0.855	0.398
VAC_centred:VIC_centred	-0.00039	0.000343	299	-1.14	0.256

Model m2.unfrozen.b, without samples in the -40 kPa matric potential treatment.

	Value	SE	df	<i>t</i> -value	<i>p</i> -value
(Intercept)	0.0647	0.156	245	0.416	0.678
VWC_centred	-0.0213	0.0165	245	-1.29	0.198
VAC_centred	-0.0564	0.0168	245	-3.36	< 0.001
VIC_centred	-0.0059	0.0156	245	-0.379	0.705
sample_groupHigh	0.232	0.289	29	0.801	0.43
sample_groupMedium	0.0629	0.207	29	0.304	0.763
VAC_centred:VIC_centred	-0.00062	0.000322	245	-1.94	0.0539

Model m3

	Value	SE	df	<i>t</i> -value	<i>p</i> -value
(Intercept)	0.194	0.184	301	1.05	0.293
unfrozen_VWC_centred	-0.00528	0.0193	34	-0.274	0.786
unfrozen_VAC_centred	-0.0497	0.0196	34	-2.53	0.016
sample_groupHigh	0.113	0.376	34	0.3	0.766
sample_groupMedium	-0.228	0.257	34	-0.886	0.382
temperature-5	-0.0529	0.021	301	-2.52	0.0122
temperature-3	-0.0582	0.0209	301	-2.78	0.00577

657 Model m4

	Value	SE	DF	<i>t</i> -value	<i>p</i> -value
(Intercept)	49.3	1.22	301	40.5	<0.001
unfrozen_VWC_centred	1.1	0.128	34	8.66	< 0.001
unfrozen_VAC_centred	0.301	0.13	34	2.32	0.0267
sample_groupHigh	2.54	2.49	34	1.02	0.315
sample_groupMedium	-0.00267	1.7	34	-0.00157	0.999
temperature-5	-2.52	0.0856	301	-29.4	< 0.001
temperature-3	-4.52	0.0854	301	-52.9	< 0.001