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Influence of Different Methods to Estimate the Soil Thermal Properties from Experimental Dataset

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Abstract: Knowledge of soil thermal properties (diffusivity (k) and conductivity (λ)) is important to understand the soil–plant–atmosphere interaction related to the physical and biological processes associated with energy transfer and greenhouse gas exchanges. The incorporation of all the physical processes that occur in the energy transfer in the soil is a challenge in order to correctly estimate soil thermal properties. In this work, experimental measurements of soil temperature and soil heat flux obtained in a silty clay loam soil covered by native grassland located in the Brazilian Pampa biome were used to estimate soil thermal properties using different methods including the influence of the soil water content at different soil depths in heat transfer processes. The λ was estimated using the numerical solution of the Fourier equation by the Gradient and Modified Gradient methods. For the surface layer, the results for both models show large variability in daily values, but with similar values for the annual mean. For λ at different soil depths, both models showed an increase of approximately 50% in the λ value in the deeper layers compared to the surface layer, increasing with depth in this soil type. The k was estimated using analytical and numerical methods. The analytical methods showed a higher variability and overestimated the values of the numerical models from 15% to 35%. The numerical models included a term related to the soil water content. However, the results showed a decrease in the mean value of k by only 2%. The relationship between thermal properties and soil water content was verified using different empirical models. The best results for thermal conductivity were obtained using water content in the surface layer ($R^2 > 0.5$). The cubic model presented the best results for estimating the thermal diffusivity ($R^2 = 0.70$). The analyses carried out provide knowledge for when estimating soil thermal properties using different methods and an experimental dataset of soil temperature, heat flux and water content, at different soil depths, for a representative soil type of the Brazilian Pampa biome.

Keywords: soil thermal conductivity; soil thermal diffusivity; soil water content; numerical modeling; Pampa biome



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1. Introduction

The numerous physical processes that occur in the soil are directly related to the complex soil–plant–atmosphere system. Knowledge of the energy transfer processes between the surface and the subsurface is fundamental for both weather and plant growth prediction models [1]. The incorporation of all the physical processes that occur in the energy transfer processes in the soil is a challenge in order to correctly estimate the soil thermal properties. The main processes of energy transfer in the form of soil heat are conduction and convection. Conduction is a process in which the energy is transferred from the region of high temperature to the region of low temperature as a result of the

random motion of molecules as in the case of fluid at rest. Convection occurs by moving fluids and is related to heat transfer mainly in moist soils [1].

Although heat transfer in soils preferentially occurs through the process of conduction, convection can make an important contribution when the soil water content increases [2]. Mathematically, these two processes would lead to a coupled system of heat and water flux [3]. The influence of soil water content can be incorporated into the heat conduction equation in solids by adding a term representing convection [4–6]. Chen and Kling [7], when studying a numerical solution for the conduction equation in solids, proposed the addition of a parameter to include the non-linear effects of all non-conductive processes present in soil temperature measurements (i.e., water flux, latent heat, water vapor flux, etc.), showing that these processes have a more significant influence on the solution in deeper layers.

The conductive and convective processes influence the soil thermal properties (thermal conductivity (λ), volumetric heat capacity (c_v) and thermal diffusivity (k)), which are also dependent on factors related to the soil type such as texture, organic matter content, mineralogical composition and soil physical structure [8]. In general, the properties are estimated from analytical solutions of the heat conduction equation in solids [9], mainly by Amplitude and Phase Shift methods [10,11] using numerical solutions such as the gradient method [12–15], or through an inverse problem solution [16].

Another challenge has been to understand the relationship between soil thermal properties and soil water content (θ) [17–22]. In general, the soil thermal conductivity increases with increasing soil moisture. In the literature, studies have presented empirical equations that describe the behavior of thermal conductivity as a function of soil water content, $\lambda(\theta)$, either relating to soil physical properties, or empirical parameters calibrated from the experimental laboratory or field data. [10,21–25]. However, few studies describe the relationship between soil thermal diffusivity and soil water content, $k(\theta)$. One such study was carried out by Arkhangel'skaya [20], who described a lognormal model of $k(\theta)$ for different soil types, using experiments carried out in the laboratory. The research indicated that the proposed model yielded better results when compared to existing ones.

In this study, we analyzed the estimation of soil thermal properties using different methods at different soil depths, including the influence of soil moisture on the energy transfer generated by the heat conduction process. Estimates were based on experimental measurements of soil temperature, soil heat flux and soil water content obtained in situ at different soil depths. The estimates for thermal conductivity were obtained from numerical solutions of the Fourier equation by the Gradient and Modified Gradient methods [8,9,15]. Soil thermal diffusivity was numerically estimated using the classical solids heat equation including a term that represents the vertical gradient of soil diffusivity related to dependence on soil water content. These results are compared with the Amplitude and Phase Shift analytical methods. The relationship between thermal properties and soil water content was evaluated through the calibration of empirical models.

This study was carried out in a natural grassland of the Pampa biome in southern Brazil used for cattle ranching, which is an economic activity of extreme importance for the regional economy [1,26]. The analyses seek to understand the thermal processes that occur locally in the Pampa biome, generating results that will contribute to the understanding of the local role in the regional context.

2. Material and Methods

2.1. Site Description and Measurements

The experimental site is located in a natural grassland intended for livestock, near the city of Aceguá, in the state of Rio Grande do Sul, Brazil (31°39'21.1" S; 54°10'30.7" W, elevation 170 m) (Figure 1a). The area is within the Brazilian Pampa biome, characterized by fields with a predominance of grasses. The typical climate of this region is classified as Cfa, according to the Köppen classification [27], defined as temperate humid with a hot summer. The annual average air temperature is 17.7 °C, which varies from up to 40 °C, in

summer (January and February), to negative values, around $-1\text{ }^{\circ}\text{C}$, in winter (June or July), and with climatic precipitation, around 1500 mm per year, well distributed between the months of the year. The soil is characterized as silty clay loam, with an average soil density of 1195 kg m^{-3} . The soil physical properties are shown in Table 1 [25,28].

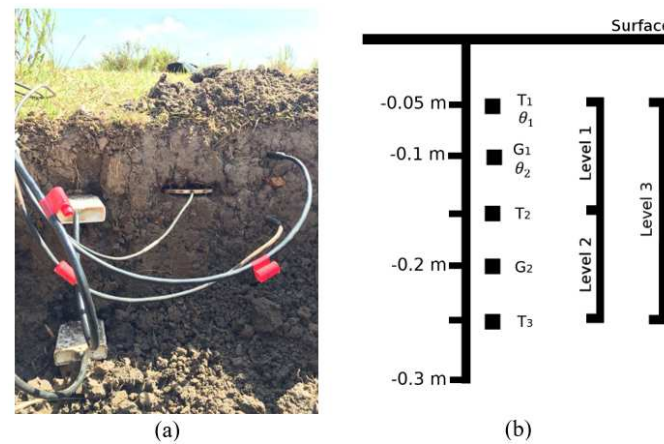


Figure 1. (a) Sensors installed in different layers in the ground at the experimental site of Aceguá-RS. (b) Position configuration of the soil sensors installed at the experimental site. G_i represents soil heat flux sensors, θ_i represents soil water content sensors for $i = 1 \dots 2$ and T_i represents soil temperature sensors for $i = 1 \dots 3$.

Table 1. Soil physical properties at the experimental site of Aceguá.

Depth (m)	Sand (%)	Clay (%)	Silt (%)	Field Capacity ($\text{m}^3 \text{ m}^{-3}$)	Permanent Wilting Point ($\text{m}^3 \text{ m}^{-3}$)	Macroporosity ($\text{m}^3 \text{ m}^{-3}$)	Microporosity ($\text{m}^3 \text{ m}^{-3}$)	Bulk Density (kg m^{-3})
0.05	16.6	35.7	47.6	0.54	0.02	0.09	0.53	930.67
0.10	14.7	39.7	45.4	0.45	0.02	0.04	0.45	1274.22
0.30	15.0	42.5	42.4	0.38	0.02	0.03	0.37	1353.63

Soil temperature (T) was measured with the T108 sensor (Campbell Scientific Inc., Logan, UT, USA) at depths -0.05 m (T_1), -0.15 m (T_2) and -0.25 m (T_3). Soil heat flux (G) was measured with the HFP01 sensor (Hukseflux Thermal Sensor B.V., Delft, The Netherlands) at depths -0.10 m (G_1) and -0.20 m (G_2), and the soil water content (θ) was measured with a CS616 reflectometer (Campbell Scientific Inc., Logan, UT, USA) at depths -0.05 m (θ_1) and -0.10 m (θ_2). A basic diagram of the sensor's installation position is shown in Figure 1b.

Data were collected in 2018 at every minute and the half-hour average was used in this study. Failures in collections are common mainly due to sensor's maintenance problems, power outages, etc. However, no failure closure methodology was performed.

2.2. Theoretical Structure

This section establishes the usual physics concepts and mathematical tools employed in the investigation of phenomena.

2.2.1. Heat Conduction Equation

The equation governing heat conduction (or diffusion) in an isotropic medium is given by the Fourier equation [9], which in the vertical direction is defined by

$$G_z = -\lambda \frac{\partial T}{\partial z} \quad (1)$$

where G_z (Wm^{-2}) is the soil heat flux, λ ($\text{Wm}^{-1}\text{K}^{-1}$) is the soil thermal conductivity, T (K) is the soil temperature and z (m) is the depth of the soil in relation to the surface. The minus sign is included to make the heat flow a positive quantity when the heat flux vector points in the direction of decreasing temperature. The one-dimensional heat conduction equation in an isotropic medium is defined in [9] as follows

$$\frac{\partial T}{\partial t} = \frac{1}{c_v} \frac{\partial G_z}{\partial z} \quad (2)$$

The differential equation describing the vertical heat flux density is obtained by substituting Equation (1) in Equation (2)

$$c_v \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(-\lambda(\theta) \frac{\partial T}{\partial z} \right) \quad (3)$$

where t (s) is the time, c_v ($\text{Jm}^{-3}\text{K}^{-1}$) is the volumetric heat capacity and θ (m^3m^{-3}) soil water content. The term on the left side of Equation (3) represents the rate of change with time of thermal energy amount contained in a soil element of volume, while the term on the right side represents the change in heat flux density along the vertical direction. Thus, it is assumed that energy exchanges occur only by conductive processes.

Assuming that the soil is thermally homogeneous (i.e., constant c_v) and defining thermal diffusivity as $k(\theta) = -\lambda(\theta)/c_v$, the estimates of the soil thermal properties were separated in the following cases:

- (i) Assuming that the soil water content is constant with respect to time and depth, then the thermal conductivity will be independent of the position; consequently, the thermal diffusivity will also be constant and, assuming these conditions, Equation (3) reduces to the particular case

$$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2} \quad (4)$$

where the soil thermal diffusivity, k (m^2s^{-1}), is independent of depth.

- (ii) Assuming that the soil water content varies depending on depth, a term including the influence of soil water content is added in Equation (2); in this case, Equation (3) can be written as follows

$$\frac{\partial T}{\partial t} = k(\theta) \frac{\partial^2 T}{\partial z^2} + \frac{\partial k(\theta)}{\partial z} \frac{\partial T}{\partial z} \quad (5)$$

Naming $\frac{\partial k(\theta)}{\partial z} = \gamma$, obtains

$$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2} + \gamma \frac{\partial T}{\partial z} \quad (6)$$

The first term on the right side of Equation (6) represents the energy transfer from the region of high temperature to the region of low temperature as a result of the motion of random molecules, while the second term includes the influence of the water content (γ term) in this process of heat transfer. The combination of these two terms expresses the speed at which the temperature variation occurs between the soil layers.

As a consequence of the assumption that thermal properties depend on θ , then they will also be position dependent; since θ is a function of depth, $\theta(z)$, so

$$\frac{\partial k}{\partial z} = \frac{\partial k}{\partial \theta} \frac{\partial \theta}{\partial z} \quad (7)$$

Therefore, the vertical gradient of thermal diffusivity depends directly on the gradient of soil moisture. The term does not represent the generation (or sink) of energy or the process of convection since the presence of water in the soil, in this case, would only indicate an increase in the heat conduction speed.

2.2.2. Heat Conduction Equation Solutions

In this work, we propose the k estimation through the analytical (Equation (4)) and numerical solution (Equation (6)), γ estimation through the numerical solution (Equation (6)) and λ from the numerical solution (Equation (1)). Soil temperature and heat flux measurements at different depths were used. The solution methods are described below.

Analytical Solution: Amplitude and Phase Shift Methods

Equation (4) can be solved analytically so that soil temperature can be described by a periodic function [8,9,29] whose temperature at a given depth (z) is defined by

$$T(z, t) = T_m + A \sin(\omega t + \varphi) \quad (8)$$

with T_m the daily average temperature, ω the angular speed of earth rotation, defined by $\omega = \frac{2\pi}{P}$, with P being the period (24 h), A the temperature amplitude and φ the phase shift (parameters to be estimated).

Soil thermal diffusivity (k) can be expressed as follows, as shown in [12]

$$k_A = \frac{\omega(z_1 - z_2)^2}{2 \left[\ln \left(\frac{A_1}{A_2} \right) \right]^2} \quad (9)$$

and

$$k_P = \frac{\omega(z_1 - z_2)^2}{2(\varphi_1 - \varphi_2)^2} \quad (10)$$

where subscript A refers to the Amplitude method (MA) and subscript P to the Phase Shift method (MPS).

Numerical Solution

The partial differential equations present in Equations (1) and (6) can be numerically solved by the centered finite difference method

$$\frac{\partial T}{\partial z} \approx \frac{T_{z_{i+1}}^n - T_{z_{i-1}}^n}{2 \Delta z} \quad (11a)$$

$$\frac{\partial T}{\partial t} \approx \frac{T_z^{n+1} - T_z^{n-1}}{2 \Delta t} \quad (11b)$$

$$\frac{\partial^2 T}{\partial z^2} \approx \frac{T_{z+1}^n - 2T_z^n + T_{z-1}^n}{(\Delta z)^2} \quad (11c)$$

where T represents the soil temperature at a given depth z , t is the time and the indices n and i represent, respectively, the temporal variation and the depth variation of the soil temperature measurement.

In this work, we use the finite difference method because it has better stability characteristics [30,31] since this method consists of replacing each of the derivatives in the differential equation with a quotient approximation of differences. The particular choice of difference quotient is carried out in such a way that a specific order of truncation error is maintained [30,31]. Thus, using the approximation of Equation (11a), Equation (1) is rewritten as

$$G_z = \lambda \left[\frac{T_{z_{i+1}}^n - T_{z_{i-1}}^n}{2 \Delta z} \right] \quad (12)$$

Equation (12) is the well-known Gradient Method (MG). Romio et al. [15] proposed a modification to the numerical solution of Equation (12), which consists of adding a constant empirical parameter (ϵ) to adjust the observed behavior of the experimental data

$$G_z = \lambda \left[\frac{T_{z+1}^n - T_{z_i}^n}{2 \Delta z} \right] + \varepsilon \quad (13)$$

Thus, Equation (13) is called Modified Gradient Method (MR).

Using the approximations of Equations (11a) to (11c), Equation (6) is solved as follows

$$\left[\frac{T_z^{n+1} - T_z^{n-1}}{2 \Delta t} \right] = k \left[\frac{T_{z+1}^n - 2T_z^n + T_{z-1}^n}{(\Delta z)^2} \right] + \gamma \left[\frac{T_{z+1}^n - T_{z-1}^n}{2 \Delta z} \right] \quad (14)$$

2.2.3. Empirical Modeling of Thermal Properties as a Function of Soil Water Content

In this paper, the behavior of soil thermal properties as a function of soil water content is analyzed using equations that fit experimental, laboratory or field data. Empirical models proposed by Tong et al. [22] and Zimmer et al. [25] are used to estimate thermal conductivity. Thermal diffusivity is estimated by Arkhangel'skaya [20], Tikhonravova and Khitrov [20] and Cubic Polynomial function (our suggestion).

Soil Thermal Conductivity as a Function of Soil Water Content

Tong et al. [22], analyzing different models in the literature, proposed the relationship

$$\lambda(\theta) = a - b.e^{(-c\theta)} \quad (15)$$

where a , b and c are empirical parameters to be estimated.

Zimmer et al. [25] used empirical adjustment equations to estimate $\lambda(\theta)$, based mainly on the curve behavior of the available experimental dataset

$$\lambda(\theta) = \lambda_{dry} + \beta.e^{\left(-\frac{\varphi}{(\theta-\theta_{min})^\alpha}\right)} \quad (16)$$

where λ_{dry} ($\text{W m}^{-1} \text{K}^{-1}$) is the thermal conductivity of a soil sample close to minimum soil moisture; the parameter β is related to the asymptotic values of the λ and also depends on the smaller value of the experimental λ (λ_{dry}); θ_{min} ($\text{m}^3 \text{m}^{-3}$) is the minimum soil moisture of the experimental dataset; $\gamma > 0$ and $\alpha > 0$ are parameters to be adjusted.

Soil Thermal Diffusivity as a Function of Soil Water Content

Arkhangel'skaya [20] describes the relationship $k(\theta)$ through the function

$$k(\theta) = k_0 + a \exp \left[-0.5 \left(\frac{\ln \left(\frac{\theta}{\theta_0} \right)}{b} \right)^2 \right] \quad (17)$$

where k_0 is the initial soil thermal diffusivity (defined by a lognormal function relation), θ_0 is the minimum soil water content and a and b are parameters to be estimated empirically.

Tikhonravova and Khitrov [20] proposed a degree 5 polynomial function described by

$$k(\theta) = a_0 + a_1\theta + a_2\theta^2 + a_3\theta^5 \quad (18)$$

where a_0 , a_1 , a_2 and a_3 are parameters to be estimated empirically.

In this study we suggest the calibration of a degree 3 polynomial function (cubic polynomial function) to evaluate the behavior in relation to the experimental data, defined by

$$k(\theta) = b_0 + b_1\theta + b_2\theta^2 + b_3\theta^3 \quad (19)$$

where b_0 , b_1 , b_2 and b_3 are parameters to be empirically estimated. Similar to the model by Tikhonravova and Khitrov [20], it is necessary to calibrate the four parameters b_0 , b_1 , b_2 and b_3 .

2.3. Evaluated Models/Methods

Soil thermal conductivity and soil thermal diffusivity were analyzed in two ways/steps: The first consisted of estimating these properties using equations that relate them to temperature and depth variation (MG, MR, MA, MPS, MN and MN_γ). The second consisted of using daily soil thermal conductivity and diffusivity data (estimated in the first step) to analyze the relationships between these properties and soil water content (MTong, MZimmer, MAk, MTK and MC).

Soil thermal properties (conductivity and diffusivity) and the vertical gradient of thermal diffusivity were estimated using experimental soil temperature data. For this, the following models/methods were used:

- MG: soil thermal conductivity (λ) estimation by the least squares method applied to the numerical solution (Equation (12)), from the daily average of the experimental data of the soil temperature.
- MR: soil thermal conductivity (λ) estimation by the least squares method applied to the numerical solution (Equation (13)), from the daily average of the experimental data of the soil temperature.
- MA: soil thermal diffusivity (k) estimation by the Amplitude (Equation (9)) analytical method. The A_1 and A_2 parameters were fitted to Equation (8) from the daily average soil temperature experimental data, using the least squares method.
- MPS: soil thermal diffusivity (k) estimation by the Phase Shift (Equation 10) analytical method. The φ_1 and φ_2 parameters were fitted to Equation (8) from the daily average soil temperature experimental data, using the least squares method.
- MN: soil thermal diffusivity (k) estimation by the least squares method applied to the numerical solution (Equation (14)), considering the γ parameter as null ($\gamma = 0$).
- MN_γ : soil thermal diffusivity (k) and vertical gradient of soil thermal diffusivity (γ) estimation by the least squares method applied to the numerical solution (Equation (14)).

Soil thermal conductivity and soil thermal diffusivity were also evaluated as a function of soil water content. To this end, the following empirical models were used:

- MTong: soil thermal conductivity estimation as a function of soil water content (Equation (15)). The empirical model proposed by Tong et al. [22].
- MZimmer: soil thermal conductivity estimation as a function of soil water content (Equation (16)). The empirical model proposed by Zimmer et al. [25].
- MAk: soil thermal diffusivity estimation as a function of soil water content (Equation (17)). The empirical–analytical model proposed by Arkhangel'skaya [20].
- MTK: soil thermal diffusivity estimation as a function of soil water content (Equation (18)). The empirical model proposed by Tikhonravova and Khitrov [20].
- MC: soil thermal diffusivity estimation as a function of soil water content, based on a Cubic Polynomial function (Equation (19)). The empirical model suggested in this research.

The daily average values of the thermal properties were estimated to analyze possible seasonality and the relationships between the properties and the soil water content using the MG and MR models for soil thermal conductivity and MA, MPS, MN and MN_γ for the soil thermal diffusivity. Three levels were considered (Figure 1): level 1 (from 0.05 m to 0.15 m); level 2 (from 0.15 m to 0.25 m); level 3 (from 0.05 m to 0.25 m). The soil thermal conductivity was estimated for level 1 and level 2, and the soil thermal diffusivity, by methods MA and MPS, in the three levels, and by MN and MN_γ in level 3 only.

The daily values of soil thermal conductivity (obtained by the MR model) and soil thermal diffusivity (obtained by the MN_γ model) were grouped at 0.01 mm intervals of the average daily soil water content for the calibration of the empirical models (MTong, MZimmer, MAk, MTK and MC) to soil water content (i.e., $\lambda(\theta)$ and $k(\theta)$). The empirical models for $k(\theta)$ analyzed in this study were calibrated only for level 3 with soil water content data measured at -0.05 m (θ_1) and the empirical models for $\lambda(\theta)$ were calibrated

for two different depth levels (levels 1 and 2) with soil water content data measured at -0.05 m (θ_1) and -0.10 m (θ_2).

To evaluate the results, the following statistical indices were used: the coefficient of determination (R^2) and root mean square error (RMSE) calculated by the following equations

$$R^2 = 1 - \frac{\sum (Y_{exp} - Y_{est})^2}{\sum (Y_{exp} - \bar{Y})^2} \quad (20)$$

$$RMSE = \sqrt{\frac{\sum (Y_{exp} - Y_{est})^2}{n}} \quad (21)$$

where Y_{exp} represents the experimental values, Y_{est} the estimated values, $\bar{Y}$ the observations mean and n the number of observations.

3. Results

3.1. Soil Variables

Half-hour averages of soil temperature (T), soil water content (θ) and soil heat flux (G), at the different measured depths, are shown in Figure 2. The lowest values for T_1 , T_2 and T_3 were 4.2 °C, 8.2 °C and 9.7 °C, in winter, and the highest were 39.9 °C, 29.5 °C and 27.2 °C, in summer, respectively. The greatest variation amplitudes throughout the day occurred in T_1 , followed by T_2 and T_3 . The seasonality between spring/summer (between 261 and 80 DOY) and autumn/winter (between 81 and 260 DOY) seasons is perceived in the three depths, but more markedly in T_1 .

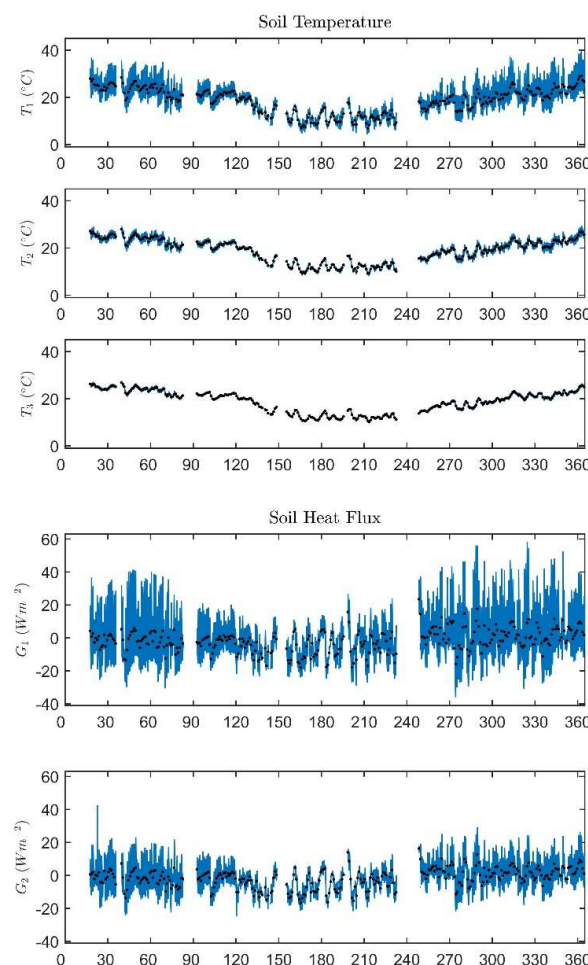


Figure 2. Cont.

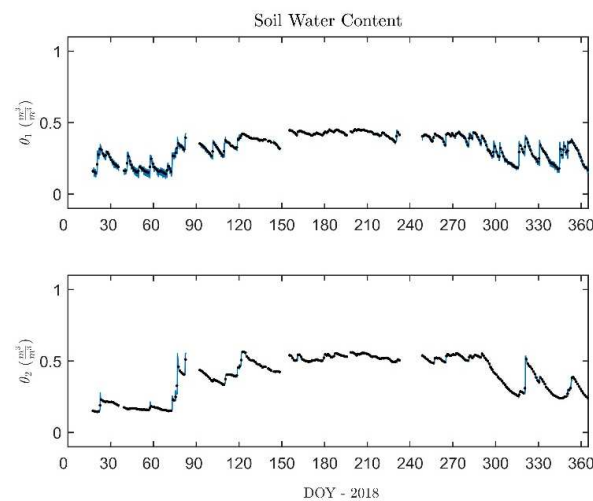


Figure 2. Measured soil temperature ($T_1 = -0.05$ m, $T_2 = -0.15$ m and $T_3 = -0.25$ m); soil heat flux ($G_1 = -0.10$ m and $G_2 = -0.20$ m); and soil water content ($\theta_1 = -0.05$ m and $\theta_2 = -0.10$ m). The blue line represents half-hour data and the black line represents daily average data.

The G showed the highest values during the spring/summer seasons for both depths, with the highest daily variability at -0.10 m (G_1). In the winter months, the daily average of G , in general, was negative; that is, the subsoil warms the surface. This result was also obtained by [25] analyzing the heat flux in a region of the same biome in southern Brazil.

The soil water content at -0.05 m (θ_1) showed variability throughout the year, with the maximum occurring between June and August. The minimum occurred in the first two months of the year, affecting even the water content at greater depths. Up to 73 DOY was considered a dry period, as the soil water content below θ_t was considered critical ($\theta_t = 0.23 \text{ m}^3\text{m}^{-3}$) according to [25,32].

3.2. Soil Thermal Properties

3.2.1. Soil Thermal Conductivity

The daily soil thermal conductivity estimated for the MG and MR methods at levels 1 and 2 are shown in Figure 3. For level 1 the λ values ranged between $0.18 \text{ Wm}^{-1}\text{K}^{-1}$ and $1.00 \text{ Wm}^{-1}\text{K}^{-1}$ to MG, whereas for MR the values were between $0.19 \text{ Wm}^{-1}\text{K}^{-1}$ and $0.84 \text{ Wm}^{-1}\text{K}^{-1}$. For level 2, the soil thermal conductivity values were between $0.15 \text{ Wm}^{-1}\text{K}^{-1}$ and $1.79 \text{ Wm}^{-1}\text{K}^{-1}$ for MG and between $0.46 \text{ Wm}^{-1}\text{K}^{-1}$ and $1.24 \text{ Wm}^{-1}\text{K}^{-1}$ for MR. It was not possible to define seasonality in the soil thermal conductivity estimates at both levels. However, MR showed less variability in the values of soil thermal conductivity for both levels analyzed. The variability observed between the results of the two models was not observed in the average values, which were similar for both models and levels analyzed. At level 1, the mean values were $0.44 \pm 0.1 \text{ Wm}^{-1}\text{K}^{-1}$ and $0.41 \pm 0.08 \text{ Wm}^{-1}\text{K}^{-1}$ for MG and MR, respectively. For level 2, mean values were $0.82 \pm 0.26 \text{ Wm}^{-1}\text{K}^{-1}$ and $0.84 \pm 0.12 \text{ Wm}^{-1}\text{K}^{-1}$ for MG and MR, respectively.

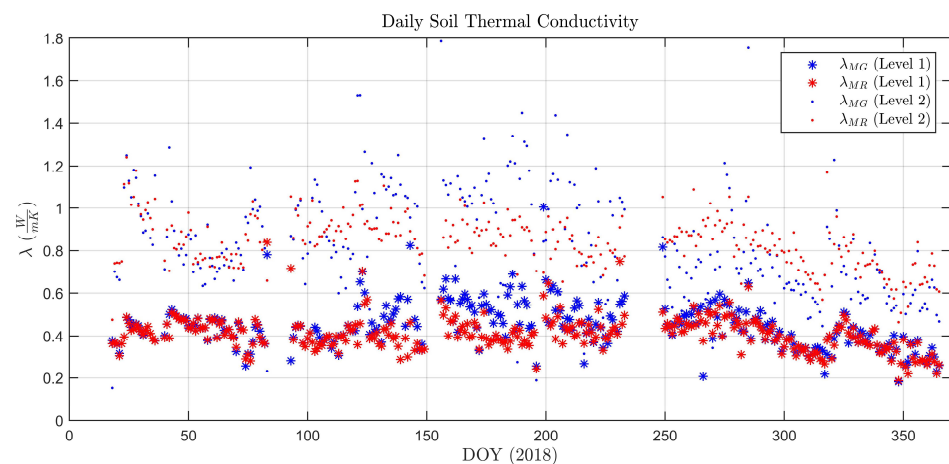


Figure 3. Daily soil thermal conductivity estimated by MG and MR models at levels 1 and 2.

The annual λ value was the same in both methods for level 1 (Table 2), while for level 2, the MR presented values around 4% higher than the MG. The results for level 1 were almost 50% lower compared to level 2, for both methods, showing that λ varies with depth. In addition, the parameter ε estimated by MR showed a difference of approximately 5 times from one level to another (difference of 2.31 W m^{-2}), being, in modulus, greater at the deepest level.

Table 2. The annual value of λ obtained from different models and different soil levels and ε obtained from the MR model.

Method	Level	$\lambda \text{ (W m}^{-1}\text{K}^{-1}\text{)}$	$\varepsilon \text{ (W m}^{-2}\text{)}$
MG	1	0.42	-
	2	0.78	-
MR	1	0.42	−0.53
	2	0.81	−2.84

3.2.2. Soil Thermal Diffusivity

The daily values of soil thermal diffusivity did not show seasonality. However, a great variability can be observed, especially for the MA and MPS methods (Figure 4a). The values obtained by MN_γ are closer to each other in a range that varies from $1.31 \times 10^{-7} \text{ m}^2\text{s}^{-1}$ to $5.91 \times 10^{-7} \text{ m}^2\text{s}^{-1}$, with a mean of $2.98 \times 10^{-7} \pm 5.33 \times 10^{-8} \text{ m}^2\text{s}^{-1}$, while those obtained by MA range from $0.40 \times 10^{-7} \text{ m}^2\text{s}^{-1}$ to $7.70 \times 10^{-7} \text{ m}^2\text{s}^{-1}$, with a mean of $3.04 \times 10^{-7} \pm 1.14 \times 10^{-7} \text{ m}^2\text{s}^{-1}$, and those obtained by MPS range from $0.73 \times 10^{-7} \text{ m}^2\text{s}^{-1}$ to $7.91 \times 10^{-7} \text{ m}^2\text{s}^{-1}$, with a mean of $3.88 \times 10^{-7} \pm 1.33 \times 10^{-7} \text{ m}^2\text{s}^{-1}$. This greater variation in the MA and MPS methods is possibly due to the simplifications. For level 3, the MA and MPS methods use the soil temperature values measured at -0.05 m and -0.25 m to estimate the diffusivity, while the MN_γ method uses the three soil temperature values measured at -0.05 m , -0.15 m and -0.25 m .

The γ parameter of the MN_γ method presented values between $-3.51 \times 10^{-6} \text{ ms}^{-1}$ and $3.22 \times 10^{-6} \text{ ms}^{-1}$, without characterizing a seasonality, according to Figure 4b, and an average γ of $1.09 \times 10^{-7} \pm 1.35 \times 10^{-6} \text{ ms}^{-1}$.

The annual values of soil thermal diffusivity (k) obtained by the MN and MN_γ methods were similar to each other and lower than those obtained by the analytical methods at the same depth interval (level 3) (Table 3). The MPS method presented the highest values, being around 30% higher than MA and 37% higher than MN and MN_γ , indicating that the method used influenced the obtained results, as also discussed by An et al. [33].

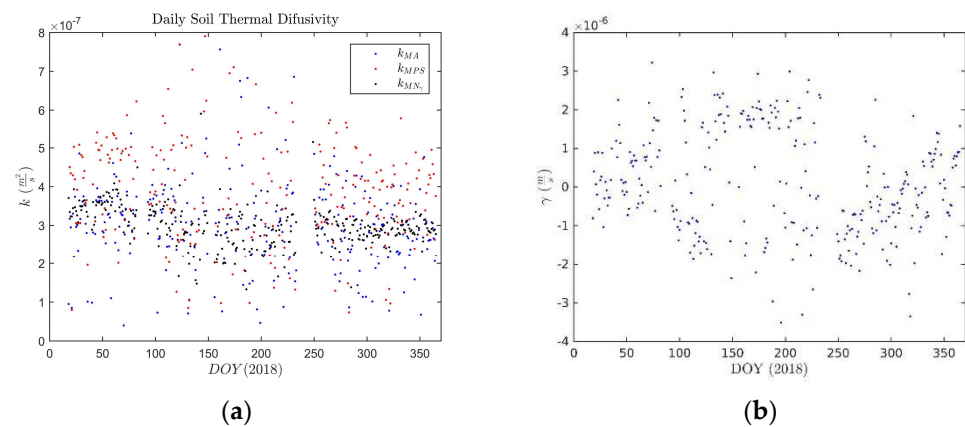


Figure 4. (a) Daily soil thermal diffusivity, level 3, estimated by three different methods: MA, MPS and MN_γ ; (b) γ obtained for MN_γ .

Table 3. The annual value of k ($\text{m}^2 \text{s}^{-1}$) and γ (m s^{-1}) for different methods and different soil levels.

Level-Layer	MN_γ		MN	MA	MPS
	(k_{N_γ})	(γ)	(k_N)	(k_A)	(k_P)
1—−0.05 to −0.15				2.90×10^{-7}	3.87×10^{-7}
2—−0.15 to −0.25				3.95×10^{-7}	5.69×10^{-7}
3—−0.05 to −0.25	2.93×10^{-7}	1.12×10^{-6}	2.98×10^{-7}	3.36×10^{-7}	4.65×10^{-7}

3.3. Soil Thermal Properties as a Function of Soil Water Content

The variations in the soil thermal properties as a function of the soil water content were analyzed through the daily values estimated by MR for thermal conductivity (λ), and by MN_γ for thermal diffusivity (k), obtained as described in Section 2.3.

3.3.1. Soil Thermal Conductivity

Figure 5 presents the values of soil thermal conductivity, obtained by MR, estimated for levels 1 and 2 distributed as a function of the average daily soil water content, including the estimates of $\lambda(\theta)$ by the calibrated models MTong and MZimmer. The MR method was chosen because it presents better results in the G estimation compared to the MG method, according to the result of [15]. There was an increase in soil thermal conductivity with increasing soil moisture but with great variability. The greatest variability was found when λ was estimated for level 2, both with soil water content at θ_1 and θ_2 .

Table 4 presents the values of the calibrated parameters and the statistical indices for the MTong and MZimmer models using the soil water content in θ_1 and θ_2 . The calibrated parameters of the models differed significantly for the different depths. Considering the soil thermal conductivity at level 1, MZimmer showed better results compared to MTong, for both depths of soil water content, with R^2 of 0.56 and 0.46, for θ_1 and θ_2 , respectively, and MTong obtaining, for the same depths, R^2 of 0.53 and 0.46, respectively. For soil thermal conductivity at level 2, it is possible to see that both models obtained similar results, highlighting that, for the relationship between soil thermal conductivity and soil water content in θ_2 , both models present extremely low statistical indices, which may be related to the higher values of soil water content at this depth. The authors of [25] found that for high values of soil water content, these models do not represent the experimental data well due to the high variability in soil thermal conductivity values.

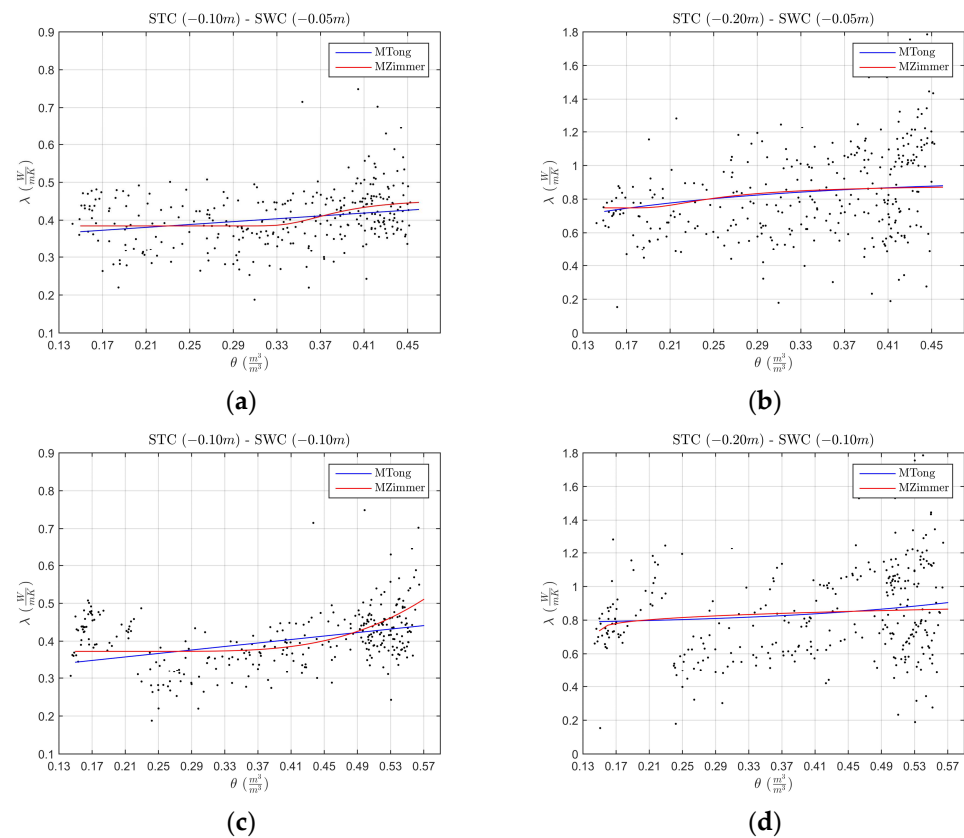


Figure 5. Soil thermal conductivity (λ) as a function of daily soil water content (θ) and the calibrated models MTong and MZimmer; (a) level 1 and θ_1 ; (b) level 2 and θ_1 ; (c) level 1 and θ_2 ; (d) level 2 and θ_2 .

Table 4. Estimated parameters from the MTong and MZimmer models and statistical indices for soil thermal conductivities at level 1 and level 2 and soil water content at θ_1 (−0.05 m) and θ_2 (−0.10 m).

	MZimmer				
	α	β	φ	R^2	RMSE
level 1— θ_1	6.39	−2.67	6.4×10^{-5}	0.56	0.021
level 1— θ_2	0.62	4.87	4.01	0.46	0.046
level 2— θ_1	1.76	−1.97	0.02	0.60	0.038
level 2— θ_2	−1.39	−2.86	−3.59	0.12	0.089
	MTong				
	a	b	c	R^2	RMSE
level 1— θ_1	3.29	2.94	0.07	0.53	0.027
level 1— θ_2	0.37	-2.51×10^{-5}	−15.45	0.46	0.046
level 2— θ_1	0.9216	0.41	4.94	0.57	0.039
level 2— θ_2	0.7675	−0.01	−4.17	0.12	0.089

3.3.2. Soil Thermal Diffusivity

The daily values of soil thermal diffusivity by the MN_γ method as a function of the average daily soil water content for θ_1 are presented in Figure 6, with the calibrated curves of the functions suggested by Arkhangel'skaya [20], MAK; Tikhonravova and Khitrov [20], MTK; and Cubic, MC. Table 5 presents the calibrated parameters and the

statistical parameters. The parameter θ_0 was obtained from experimental data of soil water content since it represents the minimum soil water content. The parameter k_0 can be obtained in two ways: analytically, when the soil physical properties are known, or numerically, in which it is calibrated along with the other model parameters. For both models, k_0 was obtained numerically. The k_0 parameter from MTK was smaller than MAK. The MTK and MC models presented better results for the estimation of the soil thermal diffusivity, with $R^2 = 0.70$, whereas MAK obtained $R^2 = 0.55$ (Table 5).

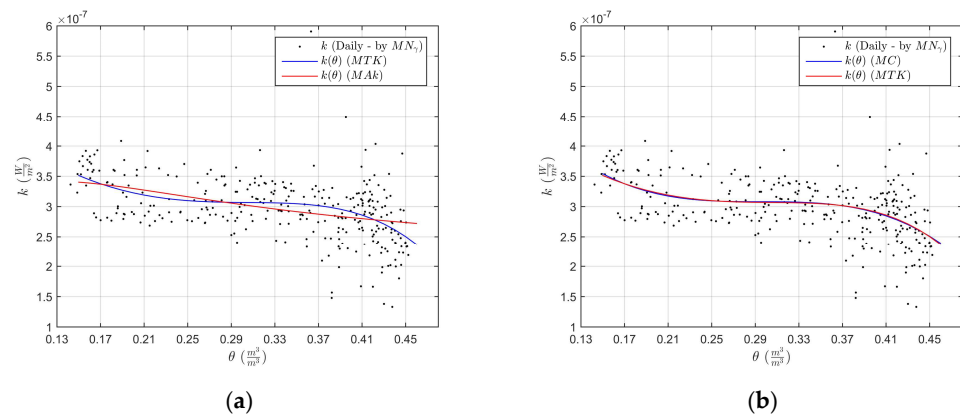


Figure 6. Daily thermal diffusivity, obtained by MN_γ (k_{N_γ}), as a function of soil water content at -0.05 m compared to: (a) MTK and MAK; (b) MC and MTK.

Table 5. Estimated parameters from Arkhangel'skaya (MAK), Tikhonravova and Khitrov (MTK) and Cubic Polynomial function (MC) models.

MAK					
k_0 (m^2s^{-1})	θ_0 (m^3m^{-3})	a	b	R^2	RMSE
2.23×10^{-7}	0.13	1.22×10^{-7}	0.92	0.55	1.94×10^{-8}
MTK					
a_0 (m^2s^{-1})	a_1	a_2	a_3	R^2	RMSE
5.60×10^{-7}	-2.05×10^{-6}	4.43×10^{-6}	-1.55×10^{-5}	0.70	1.59×10^{-8}
MC					
b_0 (m^2s^{-1})	b_1	b_2	b_3	R^2	RMSE
6.97×10^{-7}	-3.96×10^{-6}	1.34×10^{-5}	-1.52×10^{-5}	0.70	1.58×10^{-8}

However, in soils that experience evaporative drying, k tends to increase from the surface downward. The smallest value of k is at the dry surface and larger values of k occur in the moist subsurface [6,14]. The thermal diffusivity is expected to increase with humidity until reaching a “maximum” value, which is due to the increase in the effective cross-section of heat conduction with the increase in the water presence. From this, the increase in moisture does not increase the thermal conductivity and, consequently, the thermal diffusivity decreases [34].

4. Discussion

4.1. Soil Thermal Conductivity

The MG and MR models are similar solutions for solving the Fourier equation (Equations (12) and (13), respectively). However, MR includes an ε parameter whose objective is to perform a correction in the numerical solution of the heat conduction law so that the model can better adapt to the behavior observed in the experimental data of soil heat flux and soil temperature gradient [15]. As the variation in soil heat flux in relation

to the temperature gradient does not pass at the origin when evaluated in a data series, the non-inclusion of ε can generate an underestimation/overestimation in the numerical solution of soil heat fluxes. Thus, ε may be related to an energy flow not accounted for in experimental measurements, whose inclusion of this parameter influenced the lower variability in the thermal conductivity estimate, as it takes these energy fluxes into account, differently from the MG model, which showed greater variability in the daily estimate of the conductivity.

In greater depths ε was greater; that is, more energy was not captured by the measurement. The deeper in the soil the sensors were, the greater the technical problems were for installing them; that is, it becomes more difficult to guarantee that the sensors are correctly installed, mainly due to the soil being more compacted, which can be observed in the relation to the lower soil porosity (Table 1). In addition, the experimental site is used for livestock; that is, the cattle walk freely on the vegetation that is made up of grasses, and therefore, trampling contributes to soil compaction.

Soil type can influence λ values. The authors of [21], analyzing 17 different soil types, found λ values that ranged from $\sim 0.2 \text{ W m}^{-1} \text{ K}^{-1}$ to $\sim 2.3 \text{ W m}^{-1} \text{ K}^{-1}$, similar values to those obtained in this work. Furthermore, [21] indicated that this variation in λ values also occurs in the same soil type and is related to the variation in soil water content (θ).

4.2. Soil Thermal Diffusivity

Analytical methods allowed for analysis of the variation in soil thermal diffusivity with depth, showing that higher values were found at greater depths. This may be related to differences in soil porosity with depth since soil porosity influences soil water retention [2]. Ref. [33] estimated soil thermal diffusivity for different depths and different environmental conditions in a region characterized as semiarid, finding values ranging from $10^{-5} \text{ m}^2 \text{ s}^{-1}$ to $10^{-7} \text{ m}^2 \text{ s}^{-1}$. The authors of [19] estimated the soil thermal diffusivity for a clay region obtaining values in the order of $10^{-7} \text{ m}^2 \text{ s}^{-1}$. The authors of [35] estimated k for a loamy sand soil obtaining values ranging from $2.5 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$ to $8.4 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$. The authors of [7], when proposing the addition of a constant parameter, obtained values ranging from $2.8 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$ to $4.0 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$, depending on the layer under study, considering clay soil.

Considering the results of the different authors, it is possible to observe that the values estimated in this research are in agreement with the literature since they are situated in an interval from $2.90 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$ to $5.69 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$, for different methods and different depths.

4.3. Relationships with Soil Water Content

The relationship of soil thermal conductivity in relation to soil water content showed great variability, which may be related to the characteristics of the soil fraction, such as the percentage of solids, air and water, the interface between these elements and the arrangement of the solid part of the soil. Moreover, increasing porosity or air content in the soil tends to decrease conductivity, while increasing soil compaction improves thermal contact between solids and thus increases the value of thermal conductivity [2].

Soil thermal diffusivity as a function of soil water content, as well as thermal conductivity, showed great variability. Due to its relationship with conductivity, variation in one property is expected to “impact” the variation in the other. Furthermore, the increase in soil water content at greater depths may influence the non-linear effects present in soil temperature measurements.

Another relevant observation is the fact that λ and k values are affected not only by the conduction but also by the convection phenomena. This is especially evident in the period between 150 and 240 DOY when the experimental soil water content data are closest to the saturation value.

Considering the large variation evidenced between the soil thermal properties and the soil water content, it is pointed out that more field measurements would be needed

to investigate different phenomena that may interfere with the accuracy of the calibrated parameters.

5. Conclusions

In this work, we estimated the soil thermal properties, conductivity and diffusivity, for a natural grassland of the Brazilian Pampa biome through numerical and analytical models. A numerical method was proposed to estimate soil thermal diffusivity as a function of temperature at different depth levels. The estimation of the soil thermal conductivity, for the whole period, was carried out considering the MG and MR methods. For the soil thermal diffusivity, the methods MA, MPS, MN and the proposed model MN_γ were considered. The results showed that thermal conductivity and diffusivity increase with depth, in annual values, approximately 50% in conductivity and from 35% to 45% in diffusivity, from level 1 to 2. The MG model presents greater variability in the daily estimate of the conductivity, while the analytical models present greater variability for the diffusivity. The influence of the method was observed in the estimation of thermal diffusivity, with differences of around 30% between the methods.

The numerical method proposed to estimate the thermal diffusivity considered $\gamma = 0$ and $\gamma \neq 0$ (constant value) and it was found that the parameter γ contributed weakly to the estimates. Although this contribution is not so significant, it is important that the MN_γ model proposed here should be better analyzed in future experiments with a greater number of depth levels.

The model proposed by Zimmer et al. [25] for the relationship between soil thermal conductivity and soil water content showed better results, while the Tikhonravova and Khitrov [20] model and the proposed Cubic Polynomial function model showed the best results for the relationship between soil thermal diffusivity and soil water content. Finally, as mentioned, the proposed model for the relationship $k(\theta)$ (MC) presented results equivalent to MTK and better than MAK.

As a complementary part of this work, our results can be used in the verification and calibration of the Brazilian Global Atmospheric Model—BAM [36], the atmospheric component of the Brazilian Earth System Model (BESM), since no studies including soil thermal properties in southern Brazil have been carried out with this model.

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