Parametrization of soil thermal conductivity in the INM RAS-MSU land surface model

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Abstract. The land surface scheme (LSM) used in the INM RAS-MSU Earth System model is based on a simplified parameterization of heat transfer. More promising parameterizations of the thermal conductivity coefficient are selected and implemented in the computational algorithm of the model. In particular, for the first time, a fractal model of thermal conductivity is included into the LSM of global weather and climate models. It has been shown that soil surface temperature is weakly dependent on the choice of a parameterization of the thermal conductivity coefficient. The Cote-Konrad parameterization of the soil thermal conductivity coefficient can significantly improve the accuracy of reproducing heat conduction in soil.

1. Introduction

Under the conditions of global climate warming, the heat content in the active land layer increases. The main heat reservoir is the World Ocean [1], but the land also has a significant contribution in the accumulation of heat in the Earth's system [2,3]. At the same time, the pedosphere is most affected [4]. The accumulation of heat in soil causes changes in the components of the water balance, affects the formation of surface and subsurface runoff [5], the biogeochemical cycles in the soil and vegetation [6]. The thermal conductivity of soil is also important in the evolution of permafrost.

Thermal inertia of soil at depths affects the atmospheric circulation over land on time scales from weeks to several months [4]. One of the most significant thermophysical parameters of heat transfer in soil is the coefficient of thermal conductivity. Therefore, improving the parameterization of thermal conductivity of soil is important for the Earth system models.
In the active land layer block of the Earth system model of the Institute of Numerical Mathematics of the Russian Academy of Sciences (INM RAS-MSU) [7] thermal conductivity of soil is defined by a simplified parameterization of R. Pielke [8], which does not account for a number of significant physical factors. Previously it has been shown [9] that the temperature regime of bog ecosystems is not accurately obtained by the model. At the same time, in soil physics and in the physics of porous media there are a number of other methods to describe the thermal conductivity coefficient [10]. Choosing a more physically based parameterization of the soil thermal conductivity coefficient can significantly improve the simulation of heat and moisture transfer in the INM RAS-MSU model.

At the initial stage of the work, field studies were performed in the study area by the Tunkinsky Depression station of the Institute of Geography SB RAS (Irkutsk) for measuring the soil characteristics and initial vertical distribution of moisture in various types of soils. Based on the collected data, numerical experiments were performed with the INM RAS-MSU model using four selected parameterizations of the thermal conductivity coefficient in different types of soils.

2. Soil thermal conductivity models

The thermal conductivity of soil is caused by a combination and interaction of solid, liquid, and gaseous phases. Therefore, the coefficient of thermal conductivity of the soil is primarily determined by the pore space structure and the soil moisture [11]. At the same time, the soil cover is composed of various mineral components; thus, the coefficient of thermal conductivity also significantly depends on the mineralogical composition and, first of all, on the quartz content [11], which is the most heat conducting material. At the same time, it has been shown that the thermal conductivity coefficient also depends on its temperature [12,13], the pore space structure, and the particle size distribution of solids [14]. Soil density [15], salt and ion content [16], and the hysteresis temperature effect [17] have a weak influence on the thermal conductivity coefficient.

Thus, the coefficient of thermal conductivity cannot be expressed by a simple relationship. To accurately obtain its value, a comprehensive account of humidity, temperature, structural and mineralogical properties of soils is required. A number of parametrizations for soil thermal conductivity have been proposed [10]. Therefore, it is essential to choose the most physically based parameterization, which can be supplied with necessary input external parameters on the grid of the global weather or climate model.

In the basic version of the INM RAS-MSU model, the coefficient of soil thermal conductivity \( \lambda_T \) is given by the formula of R. Pielke [8], where the soil moisture content factor is accounted through the function of the soil moisture potential \( \psi \):

\[
\lambda_T = 418.7 \max(\exp(-P_f - 2.7), 0.00041), \quad P_f = \log_{10}(-\psi). \quad (1)
\]

The value of the soil moisture potential is based on the empirical relation [17]:

\[
\psi = \psi_{max} \left( \frac{W_{max}}{W} \right)^b,
\]

where \( W \) is the ratio of the liquid moisture mass to that of dry soil, kg/kg; \( W_{max} \) is the maximum moisture content in the soil layer, kg/kg; \( b \) is a dimensionless Clapp–Hornberger parameter, which is determined by the soil type. The maximum moisture content of soil depends on the values of dry soil density \( \rho_d \) and porosity \( \Pi \).

This relationship is empirical, and the type of soil and the amount of liquid moisture are not accounted explicitly. Porosity, density, structural features, and mineralogical composition have only an indirect effect through the soil classification used in the model.

As a rule, the thermal conductivity coefficient models are based on a theoretical form, which is calibrated by the results of field experiments [10]. The most common approach in the modern soil science to predict the coefficient of thermal conductivity of soils is based on a geometric mean method of the values of the coefficient of thermal conductivity which, for three phases present in the soil, can be written as:
\[ \lambda_T = \lambda_s^{1-n} \lambda_w^{n} \lambda_a^{S_r x (1-S_r)} x \Pi, \]

where \( \lambda_s \), \( \lambda_w \), and \( \lambda_a \) are the coefficients of thermal conductivity of the solid phase of the soil, water, and air, respectively; \( S_r \) is the degree of soil saturation. However, for unsaturated soils this theoretical formula has a weak agreement with experimental data, and that is why the concept of normalized thermal conductivity was introduced in [19], where the normalized conductivity is

\[ k_r = \frac{\lambda_T - \lambda_{dry}}{\lambda_{sat} - \lambda_{dry}}. \]

The thermal conductivity of saturated soil is also given by a geometric mean

\[ \lambda_{sat} = \lambda_w^{n} \lambda_s^{1-n}, \]

and the thermal conductivity of dry soil is expressed by the empirical relationship

\[ \lambda_{dry} = \frac{A \rho_d + B}{\rho_s - C \rho_d}, \]

where \( \rho_d \), \( \rho_s \) are the dry density of soil and the density of solids, respectively; \( A=0.137, B=64.7, C=0.947 \) are empirical coefficients. The normalized thermal conductivity can be set in terms of the degree of saturation [20]:

\[ k_r = 0.7 \log(S_r) + 1, \text{ (for sands)} \]
\[ k_r = S_r, \text{ (for loam soil)}. \]

Applying the dependencies (5)-(8), the coefficient of thermal conductivity of the soil can be expressed as follows:

\[ \lambda_T = \left( \frac{\lambda_{dry} \lambda_{sat}^{1-n} - \frac{A \rho_d + B}{\rho_s - C \rho_d}}{\rho_s - C \rho_d} \right) \lambda_{sat} + \frac{A \rho_d + B}{\rho_s - C \rho_d} \]

This model is commonly referred to as the Johansen model and uses parameters that can be expressed in terms of soil porosity and density, but the mineralogical composition of soils and their granulometric typing are not explicitly accounted. From this point, the Cote and Konrad model [21] is more comprehensive, which follows the concept of “normalized thermal conductivity” as well, as in equation (5), but takes into account more explicitly the soil type and the pore space structure:

\[ \lambda_d = \chi 10^{-\eta n}, \quad k_r(S_r) = \frac{C S_r}{1 + (C - 1) S_r}, \]

where \( \chi \) and \( \eta \) are empirical coefficients determined by the soil type and the grain radius distribution; \( C \) defines the function \( k_r(S_r) \) and is soil-type specific.

It is well-known that the Johansen and Cote-Konrad models reproduce the measured values of the soil thermal conductivity coefficient with a good accuracy [10]; they have a physically profound theoretical basis and use the soil properties available from field measurements. Therefore, these models were chosen for implementation in the numerical algorithm of the active land layer model of the INM RAS-MSU.

There are also models for calculating the thermal conductivity coefficient developed in thermohydrodynamics of porous media. For instance, the fractal model for the thermal conductivity coefficient [22] is based on Fourier's law of thermal conductivity applied to individual soil particles, and then averaged over all grains of sample volume given their distribution by size. The main concept of the method is using the distribution of solid soil particles by size based on the fractal scaling law:

\[ -dN = D_f s \frac{D_f s_{r_{min}}^{D_f s}}{r_{min}^{D_f s + 1}} dr, \]

where \( r \) is the diameter of solid soil particles. To describe the microstructural features of soil grains and the presence of liquid phase in the pores, the corresponding fractal dimensions \( D_{fs} \) and \( D_{fw} \) were introduced:

\[ D_{fs} = D_E - \frac{\ln(1 - \Pi)}{\ln(r_{min}^{D_{fs}})}, \quad D_{fw} = D_E - \frac{\ln \Pi}{\ln(\varepsilon_{min}/\varepsilon_{max})}. \]
where $r_{\text{min}}, r_{\text{max}}$ are the minimum and maximum diameters of soil particles, $D_E = 3$ is the Euclidean dimension, $\Pi_\text{w} = S_\Pi \Pi$ is the volume fraction of the liquid phase in soil; and $\varepsilon_{\text{min}}, \varepsilon_{\text{max}}$ are the minimum and maximum pore diameters. Similarly, a tortuosity fractal dimension of the liquid phase $D_{T\text{w}}$ is introduced. Based on equations (11) – (12), an expression for the effective thermal conductivity of unsaturated porous media can be written as:

$$
\lambda_T = \gamma + \beta \frac{\nu (\lambda_s - \gamma)}{\lambda_s + 2\gamma}
$$

(13)

where the coefficients $\alpha$, $\beta$, and $\gamma$ have the following form:

$$
\alpha = \frac{D_{T\text{w}} + D_{f\text{w}} - 1}{D_{f\text{w}}} \left(1 + \frac{D_{T\text{w}} - 1}{D_{f\text{w}} - D_{T\text{w}}}ight), \quad \beta = \frac{3(3-D_{f\text{w}})^2}{D_{f\text{w}}^2(3-D_{f\text{w}})}, \quad \gamma = [\alpha \lambda_w + (1 - \alpha) \lambda_d].
$$

(14)

Only the porosity and moisture content of the soil are required as input data, and the type of soil can be considered through the thermal conductivity of the mineral part. However, previously it has been shown [23,24] that the values of $\varepsilon_{\text{min}}/\varepsilon_{\text{max}}$ and $r_{\text{min}}/r_{\text{max}}$ do not have a strong dependence on the particular soil types and should be determined for each individual profile. Therefore, these parameters might be considered as calibration parameters, but they limit the utilization of the parameterization on the global grid of the weather and climate model.

3. Materials and methods

To improve the quality of simulation of heat and moisture transfer, the model requires accurate information about the initial vertical distribution of soil moisture and the thermophysical parameters included in the methods for calculating the thermal conductivity coefficient. For this, in August 2019 field studies were conducted in the Tunkinsky depression in the Republic of Buryatia. A distinctive feature of this area is a variety of soil types in a limited area [25]. The bottom of the basin in its middle part is characterized by homogeneous meteorological conditions [26], and the presence of a meteorological station in the Tunka village makes it possible to obtain the necessary boundary conditions for the model, i.e. the conventional weather variables. Thus, it can be assumed that the differences in the vertical distribution of temperature and humidity between sites are caused only by the thermophysical properties of the soil and its surface. Also, in the Tunkinsky Depression, the Institute of Monitoring of Climate and Ecological Systems SB RAS (Tomsk) and the Sochava Institute of Geography SB RAS (Irkutsk) conduct unique temperature measurements at depths of up to 10 meters in various types of soils.

During the field study, the values of density, porosity, and initial moisture distribution were obtained at depths of up to 50 cm (0-10 cm, 10-20 cm, 20-30 cm, 30-40 cm, 40-50 cm) for 7 points within the valley, as shown in Figure 1. These points are characterized by the openness of terrain, so that high vegetation had almost no effect on short-wave radiation coming to the soil surface. At the same time, all points differ in soil types and features of the structure of soil profiles.

Figure 1. Geographical location of the points with thermistor strings over the Tunkinsky depression.
Each of the studied points is equipped with atmospheric-soil measuring complexes (ASMC) [27], which are scythes with temperature sensors located at intervals of 5-10 cm. The equipment allows one to obtain detailed temperature profiles in the soil with a measurement error of ±0.1 °C [28]. The time step of measurements is 1 hour.

For the considered soil sites, there is no detailed information about the mineralogical composition of the soil. Therefore, the profiles were conditionally divided by the granulometric composition of the soil into 3 types: loam, sandy soils, and peat (organic) soils. The convenience of this division is due to the fact that empirical coefficients and dependencies are specified for them individually in the Johansen [20] and Cote-Konrad [21] parameterizations.

Based on the collected data, a series of numerical experiments was performed with the INM RAS-MSU land surface model: for each soil column, a time series of soil temperature values was simulated using each of the above-described parameterizations of the thermal conductivity coefficient. The simulation was performed for the beginning of August 2019 with a time step of 1 hour. The modelling period covered 7 to 8 days for various points. The simulation results were compared with the ASMC temperature profiles.

4. Results and discussion

Temporal variability is reproduced satisfactorily when using all parameterizations of the thermal conductivity coefficient in different types of soils. At the same time, the surface temperature values weakly depend on the parameterization of the soil thermal conductivity. For wet peat bog soil (Figure 2), it is noticeable that according to the Pielke model the coefficient of thermal conductivity is significantly overestimated, which leads to an overestimation of the amplitude of temperature fluctuations in the daily course at different depths. Thus, the use of the Pielke parameterization leads to errors in reproducing heat transfer under conditions of high moisture content in soil.

Model errors in the temperature simulation noticeably decrease with depth (Figure 3). As a rule, at levels of 30 cm and below, the value of model errors approaches the level of measurement error (0.1°C). Maximum errors are observed near the surface, which is due to inaccuracies in the simulation of the heat balance and net radiation of the surface.

![Figure 2](image_url). Time series of temperature at various depths for peat bog soil according to measurements and simulations using different models for thermal conductivity.
To exclude the influence of the heat balance error on the surface, a new metric was introduced to quantify the model performance. According to the Fourier law of thermal conductivity, the ratio of the temperature amplitude at each level $\sigma_i$ to the oscillation amplitude at the surface $\sigma_s$ is determined solely by the value of the thermal diffusivity coefficient. In this case, the quality of the model's representation of the thermal conductivity coefficient is determined by the proximity of the vertical distribution $\sigma_i/\sigma_s$ to the profile of the same metric for the observation data.

For all types of soils (Figure 4), the Pielke parameterization did not produce the most accurate results. The choice of Cote-Konrad parameterization allows one to obtain most reliable results in loam and sandy soils. High accuracy of the temperature simulation was achieved by using the fractal model of thermal conductivity for moisture-saturated organic soil.
Thus, it has been shown that the R. Pielke parametrization used in the basic version of the INM RAS-MSU model is less accurate than the more modern parametrizations of thermal conductivity. The fractal model of thermal conductivity has a good potential for improving the accuracy of temperature simulations, but its use is limited in global models of weather and climate by the lack of global databases for some of its parameters. For the INM RAS Earth System model, the Cote-Konrad parametrization [21] of the soil thermal conductivity coefficient is recommended. More physically based parametrizations can improve the simulation of heat transfer with the INM RAS-MSU land surface model.

Acknowledgments
The calculation experiment was supported by the Ministry of Science and Higher Education of the Russian Federation under project AAAAA-A17-117013050037-0, the other parts of the study were supported by the Russian Foundation for Basic Research under projects no. 20-05-00773, no.18-05-00306, and no. 20-04-00142.

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