Modeling the temperature and humidity conditions of mineral soils in an active layer model taking into account in depth changes in the thermodynamic properties of the soil

V Yu Bogomolov¹², E A Dyukarev E¹², V M Stepanenko³⁴⁵ and E D Drozdov⁴

¹Institute of Monitoring of Climate and Ecological Systems, Siberian Branch of the Russian Academy of Sciences, 10/3 Akademicheskiy Ave., Tomsk, Russia
²Moscow Center of Fundamental and Applied Mathematics, Leninskie Gory 1, bld.1, Moscow, Russia
³Yugra State University
⁴Moscow State University, Faculty of Geography, Leninskie Gory 1, bld.1, Moscow, Russia
⁵Moscow State University, Research Computing Center, Leninskie Gory 1, bld.4, Moscow, Russia

Bogomolov@scert.ru

Abstract. The thermal regimes of peat and mineral soils differ significantly. Peat soils are characterized by the presence of a surface peat horizon, which is replaced by organogenic rock. The total thickness of the peat layer can reach several meters. The peat strata is a complex organomineral system with specific properties: high water content and porosity, the content of a large amount of little decomposed organic. For the correct modeling of this type of soil, a transition was made from the approach of modeling heat and moisture transfer in a porous medium with averaged thermodynamic characteristics (porosity, density, hydraulic conductivity...), to modeling heat and moisture transfer for each of the identified soil types with individual properties. In addition, in the modified model, all constants describing the thermodynamic properties of the soil are functions of depth. This made it possible to model soils with a complex soil profile, for example, bog ecosystems (peat deposit and a layer of mineral soil under it). To calculate the thermophysical characteristics of soils, the measured volumetric content of organic matter, mineral particles of different sizes, and soil porosity at all depths were used. Calculations based on the model of the active layer showed that within the framework of the approach used it is possible to correctly reproduce heat and moisture transfer in both mineral and organic soils without adding any runoff-related parameterizations, but using relevant thermophysical characteristics of the soil.

1. Introduction

An important stage in the development of a model of the active land layer is correct representation of changes in the mineral composition of the soil in depth, which is consistent with the types of existing landscapes above and the related thermophysical characteristics, and the transition from modeling of heat and moisture transfer in a porous medium with averaged thermodynamic characteristics of the soil types in a cell (porosity, density, hydraulic conductivity ...) to simulating heat and moisture transfer for each of the selected types with individual properties and already aggregated flows from the surface over them to obtain average values for the cell.

This evolutionary stage, together with the transition from the basic system of equations for temperature, moisture, and ice to a system in which all constants describing the thermodynamic
properties of the soil become functions of depth, allows modeling of soils with very different properties in depth, for example, bog ecosystems. It should be stressed that in the vast majority of models the soil properties do not change with depth. The consideration of such components of the active layer as wetland ecosystems, in addition to the thermodynamic properties of the soil, entails a correct reproduction of the land hydrological cycle in modeling the entire Earth system, which has a huge fundamental and applied importance. Soil moisture significantly affects the components of radiation balance between the apparent and latent heat fluxes and, thus, the diurnal course of deep convection in summer [2].

In order to simulate heat and moisture transfer in the soil, in addition to boundary conditions, initial conditions are necessary. Initial distributions of moisture and thermal characteristics of the soil can have a decisive influence on the thermal regime of soil cover. Therefore, at the initial time it is necessary to know with sufficient accuracy the in-depth distribution of the soil temperature, as well as the amounts of liquid and frozen moisture in the fractions of dry soil. The initial temperature and humidity profile can be determined from measurement data, and the ice content in the pore space of the soil in July can be set to zero. The calculation period is 8 years, 2011-2018, being the same as the measurement period.

An analysis of the results shows that to reproduce the temperature regime of bog ecosystems it is not enough just to introduce a new type with its hydrodynamic properties, it is necessary to switch to the hydrodynamic properties of soil as a function of depth for a correct reproduction of bogs with any depth of peat deposits. Moreover, the results obtained allow us to state that in cases of oligotrophic bogs the groundwater level can be reproduced correctly without adding any parameters related to the runoff.

A correct representation of changes in the mineral composition of soils with respect to depth is an important stage in the development of a model of the active layer of land to match the types of existing landscapes above them and the accompanying thermophysical characteristics. This is needed to model heat and moisture transfer for each of the selected types with individual properties for further aggregation of flows from the surface to obtain average values for the cell.

Consideration of the active layer components such as bog ecosystems, in addition to the thermodynamic properties of the soil, entails correct reproduction of the hydrological cycle of the land within the framework of modeling the Earth system which, in turn, is of great fundamental and applied importance. Soil moisture significantly affects the distribution of the radiation balance components between the fluxes of sensible and latent heat and, thus, the diurnal variation of deep convection in summer [2].

2. Methodology
One of the goals of this work is to reproduce the temperature regime of organic soils, for which it is necessary to take into account the effect of the organic matter content on the soil characteristics. In [1], [7] it is proposed to calculate the thermophysical characteristics of the soil (heat capacity, thermal conductivity, porosity, etc.) as a linear combination of these parameters for mineral and organic soils, taking into account the mass content of the amount of organic matter. For porosity, the following ratio is proposed:

$$\Pi = (1 - f_{om})\Pi_{min} + f_{om}\Pi_{om}$$

where $f_{om}$ is the volumetric content of organic matter in the soil layer, $\Pi_{min}$, $\Pi_{om}$ is the porosity of the mineral and organic parts of the soil. We have applied this approach to determining the density, porosity, and volumetric heat capacity of the soil in a modified form.

The volumetric heat capacity of the soil is calculated as the total heat capacity of the environments of its components:

$$c = (1 - \Pi)c_z + (\Pi - W - I)c_{vap} + Wc_{wat} + Ic_{ice},$$
where \( \Pi \) is the porosity, \( 1 - \Pi \) is the volume fraction occupied by the solid phase, \( W \), \( I \) are the volumetric moisture and ice content. The solid phase of the soil consists of five components: gravel \( (v_{grav}) \), sand \( (v_{sand}) \), silt \( (v_{silt}) \), clay \( (v_{clay}) \), which add up to the mineral phase of the soil \( (v_{min}) \) and the organic matter \( (v_{org}) \) of the soil,

\[
v_{min} + v_{org} = 1; \quad v_{grav} + v_{sand} + v_{clay} + v_{silt} = 1.
\]

Assuming that the density of the soil mineral particles \( (\rho_{min} = 2700 \text{ kg/m}^3) \) as well as the organic matter \( (\rho_{om} = 1500 \text{ kg/m}^3) \) is known, we can determine the soil density through porosity:

\[
\rho = (1 - \Pi)(v_{min}\rho_{min} + v_{om}\rho_{om}).
\]

The heat capacity of the solid phase of the soil depends on the organic matter content and the mineral component:

\[
c_s = c_{SM}v_{min} + c_{SO}v_{org}.
\]

For mineral soil, the heat capacity of the soil is related to the content of coarse and fine fractions [3]:

\[
c_{SM} = \frac{2.128 v_{sand} + 2.385 v_{clay}}{v_{sand} + v_{clay}},
\]

which is about \( 2.1-2.3 \times 10^6 \text{ J/m}^3/\text{K} \) for clays and sands, and the heat capacity of organic matter is slightly higher and is equal to \( 2.5 \times 10^6 \text{ J/m}^3/\text{K} \).

The thermal conductivity coefficient of the soil is determined by the interaction of the solid, liquid, and gaseous phases of the soil; therefore, it essentially depends, first of all, on its moisture content [4]. Moreover, this relationship cannot be approximated by one function, and changes depending on the soil saturation with moisture. Thus, at low values of moisture in the soil the molecular mechanism of heat transfer predominates and the thermal conductivity coefficient changes little. With an increase in moisture, vapor-diffusion heat transfer develops, and an exponential increase in the thermal conductivity coefficient is observed depending on the soil moisture. However, in soils saturated with moisture the vapor diffusion transfer is weakened and heat exchange is reduced to convection, which is extremely weakly expressed in soils; as a result of this the increase in the thermal conductivity coefficient practically stops.

Thus, the thermal conductivity of soils is determined by a number of moisture, density, and temperature factors, which is expressed in the possibility of determining the thermal conductivity coefficient through various quantities characterizing these dependencies. The construction of such dependencies is expressed in various ways of parameterizing this characteristic.

In the new version of the model of the active layer of land to calculate the coefficient of thermal conductivity, we use a modified Johanssen model [5], where the thermal conductivity of moist soil depends on the presence of moisture and ice and organic matter,
3. Input Data and Results

A significant modification of the model is the transition from the approach of modeling heat and moisture transfer in a porous medium with averaged thermodynamic characteristics of soil types in a cell (porosity, density, hydraulic conductivity ...) to modeling heat and moisture transfer for each of the selected soil types with individual properties and already aggregating flows from the surface over them to obtain average values for the cell. Moreover, in the modified model all constants describing the thermodynamic properties of soil are functions of depth. This made it possible to model soils with a complex soil profile, for example, bog ecosystems (a peat deposit and a layer of mineral soil under it). At the same time, it should be understood that prior to this the model did not include such a type as peat or soil close to it in terms of hydrodynamic properties. Within the framework of this work, it was necessary to understand whether it is possible within the framework of the approaches and parameterization to reproduce the temperature and humidity regime, both in mineral and peat soils, only by varying the soil parameters responsible for its hydrodynamic and thermophysical properties.

To calculate the thermophysical characteristics of soils it is necessary to know the volumetric content of organic matter, mineral particles of different sizes, and soil porosity at all depths. For our model, we recalculated the soil parameters [6] specified for depths of 0–0.0175, 0.0175–0.0451, 0.0451–0.0906, 0.0906–0.1655, 0.1655–0.2891, 0.2891–0.4929, 0.4929–0.8289, 0.8289–1.3828, 1.3828–2.2980, and 2.2980–3.8019 m for depths of 0.01, 0.02, 0.04, 0.08, 0.15, 0.25, 0.35, 0.45, 0.55, 0.65, 0.75, 0.85, 0.95, 1.05, 1.15, 1.25, 1.35, 1.45, 1.55, and 2 m using cubic spline interpolation. At depths of 3.5 and 10 m the soil characteristics were set equal to the characteristics of the lower layer (2.2961–3.8019 m) from the database.

As you can see in Figure 1 shows the soil density distribution and the grain-size composition for grid cells located along the meridian 80° E at different latitudes. As we can see, in Western Siberia (cells 55 and 60° N), a large amount of organic matter appears in the upper part of the soil profile, which corresponds to peat bogs. In the tundra zone (65° N), the thickness of the organogenic soil layer decreases.

![Figure 1](image-url)

**Figure 1.** Profiles of the distribution of soil characteristics in depth at grid nodes with coordinates 45° N, 50° N, 55° N, 60° N, and 65° N. Volumetric content of gravel (1), sand (2), dust (3), clay (4), organic matter (5) - upper axis. Soil density (6) - bottom axis.
For the study of the soil temperature regime, the thermophysical characteristics were determined from the results of a study of soil and peat samples. A layer of peat about 200 cm thick is underlain by dense clays. The content of mineral particles in the peat is small, and the properties of the soil are completely determined by the porosity of organic matter. The density of the upper layers of peat is low, and it is in good agreement with the results of field studies. The density and porosity of the peat increase with depth, and at depths of 240 and 320 cm the density and porosity correspond to the parameters for clay.

Calculations based on the model of the active layer showed that within the framework of the approach used it is possible to correctly reproduce heat and moisture transfer in both mineral and organic soils without adding any runoff-related parameterizations, but only by changing the thermophysical characteristics of the soil with depth. Two model experiments were performed. External parameters (air temperature, incoming solar radiation, precipitation intensity, etc.) were set according to observations at the Bakchar meteorological station, and were the same in both experiments. The results of model calculations were compared with the results of field observations of soil temperature (clay-OBS, peat-OBS) (Figure 2). The calculations were carried out for 2012-2017 with a time step of 1 hour, and to ensure the acceleration of the model the calculation for the first two years did not participate in assessing the model accuracy.
Figure 2. Time variation of average daily soil temperature according to observation and modeling data for 2011-2017 at depths of 20 (a), 60 (b), 80 (c), 160 (d) and 240 (e) cm. 1-clay, model; 2-peat, model; 3-clay, observation; 4-peat, observation.

The surface temperature in the active layer is completely determined by the atmospheric action in both experiments. Despite the fact that the largest error in the calculations was obtained for the surface layer, in comparison with the observational data the correlation coefficient between the observed and model values is very high. For heavy loamy soil, the absolute error decreases with depth; however, for depths of 160 and 240 cm the synchronicity of fluctuations between the model and observed values decreases, which is manifested in a decrease in the correlation coefficient. Analysis of model calculations for peat soil showed a high correlation between the model and observed temperature values. As in the case of heavy loamy soil, the absolute error decreases from the surface to a depth of 30 cm, after which the error increases. The in-depth discrepancies in the reproduction of the observed temperatures are associated with the insufficiently accurate soil properties and reproduction of the groundwater level, which affects the inertia of heating and the processes of thawing and freezing.

The depth of seasonal freezing is reproduced quite correctly. For clay it is about 90 cm, and for peat 30 cm. At a depth of more than 60 cm both types of soil are completely saturated with water, which is typical for the West Siberian Lowland.

A detailed examination of a moisture profile (Figure 3) which is obtained as a result of the calculations shows that correct accounting for the distribution of organic matter in depth allows one to correctly reproduce important characteristics of bog ecosystems significantly different from mineral soils.

Figure 3. Soil temperature and moisture profile for clay and peat.

Analysis of the results shows that to reproduce the temperature regime of bog ecosystems it is not enough just to introduce a new type with its hydrodynamic properties; it is necessary to take into account the changes in the hydrothermal properties of the soil with depth and use adequate maps of reproduction of bogs with data on the thickness of the peat deposit. The results obtained allow us to
assert that in the case of oligotrophic bogs the groundwater level can be correctly reproduced without adding any parameters related to the runoff.

4. Acknowledgments
The calculation experiment was supported under RFBR 18-05-00306 and RFBR 20-05-00773 grants. The other part of the study was supported by the Ministry of Science and Higher Education of the Russian Federation under project no. AAAA-A17-117013050037-0.

References
[1] Lawrence D M, Slater A G, Tomas R A, Holland M M and Deser C 2008 Accelerated Arctic land warming and permafrost degradation during rapid sea ice loss Geophys. Res. Lett. 35
[2] Cioni G and Hohenegger C 2017 Effect of Soil Moisture on Diurnal Convection and Precipitation in Large-Eddy Simulations J. Hydrometeorol 18 (7) 1885–903
[3] Farouki OT 1981 Thermal properties of soils CRREL Monograph 81 (1)
[4] Shein EV 2005 A course in soil physics (Moscow: Moscow University Publishing House) 432 p
[5] Johansen O 1975 Thermal conductivity of soils (CRREL Draft English Translation) 637 p
[6] Dai Y, Shangguan W, Wei N, Xin Q, Yuan H, Zhang S, Liu S, Lu X, Wang D and Yan F 2019 A review of the global soil property maps for Earth system models SOIL 5 137–58
[7] Willeit M and Ganopolski A 2018 The importance of snow albedo for ice sheet evolution over the last glacial cycle Climate of the Past 14 697-707