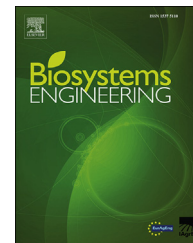




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journal homepage: www.elsevier.com/locate/issn/15375110**Special Issue: Numerical Tools for Soils****Research Paper****Estimating soil thermal diffusivity at different water contents from easily available data on soil texture, bulk density, and organic carbon content**

Tatiana Arkhangelskaya*, Ksenia Lukyashchenko

Faculty of Soil Science, Lomonosov Moscow State University (MSU), Leninskie Gori 1-12, 119991 Moscow, Russian Federation

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This study provides an algorithm to estimate soil thermal diffusivity at any water content from data on soil texture, bulk density, and percentage of organic carbon. Models were trained on the dataset of 77 soil samples including silty clays, silty clay loams, silt loams, clay loams, loams, sandy clay loams, sandy loams, loamy sands, and sands. The ranges of sand, silt, and clay within the dataset were 1–97, 2–80, and 1–52%; wet bulk density varied from 860 to 1820 kg m⁻³, organic carbon ranged from 0.1 to 6.5%. Thermal diffusivity of the undisturbed soil cores measured by the unsteady-state method was from 0.77 to 10.09 × 10⁻⁷ m² s⁻¹. The dataset was split randomly into the training set of 67 samples and the test set of 10 samples; the procedure was repeated three times. Models were developed from the measured thermal diffusivity vs. water content curves. The experimental data points for each sample were described by a 4-parameter function. Parameters of average curves for different textural classes were also determined. Then regression equations were obtained to estimate the parameters of the thermal diffusivity vs. water content function for different soils: (i) from soil texture; (ii) from soil texture and bulk density; (iii) from soil texture and organic carbon; (iv) from soil texture, bulk density, and organic carbon. The test set data were used to evaluate the model performance. The normalised root mean square errors of the best-performing models were from 20 to 33% depending on soil information available.

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1. Introduction

Thermal diffusivity is equal to thermal conductivity divided by volumetric heat capacity and reflects both the soil ability to

transfer heat and its ability to change temperature when heat is supplied or withdrawn. The higher soil thermal diffusivity is, the thicker is the soil/ground layer in which diurnal and seasonal temperature fluctuations are registered, and the smaller are the temperature fluctuations at the soil surface.

* Corresponding author.

E-mail addresses: arhangelskaia@gmail.com (T. Arkhangelskaya), Soil.lks@gmail.com (K. Lukyashchenko).<http://dx.doi.org/10.1016/j.biosystemseng.2017.06.011>

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Nomenclature

| | |
|------------|--|
| a | parameter of the $\kappa(\theta)$ function; difference between the highest thermal diffusivity and the thermal diffusivity of dry soil, $\text{m}^2 \text{s}^{-1}$ |
| AC-model | average curve model |
| AIC | the Akaike information criterion |
| b | parameter of the $\kappa(\theta)$ function; peak width, dimensionless |
| C | organic carbon content, % by mass |
| Clay | clay content, % by mass |
| d_r | the Willmott's index of agreement |
| k | number of predictors |
| n | number of cases |
| NRMSE | normalised root mean square error, % |
| \bar{O} | mean experimentally observed value of soil thermal diffusivity within the test set, $\text{m}^2 \text{s}^{-1}$ |
| O_i | observed (measured) thermal diffusivity from the test set, $\text{m}^2 \text{s}^{-1}$ |
| P_i | model-predicted thermal diffusivity from the test set, $\text{m}^2 \text{s}^{-1}$ |
| R^2 | determination coefficient |
| RMSE | root mean square error, $\text{m}^2 \text{s}^{-1}$ |
| RSS | residual sum of squares, $\text{m}^4 \text{s}^{-2}$ |
| sand | sand content, % by mass |
| SG-models | sand group models |
| silt | silt content, % by mass |
| TC-models | textural class models |
| U-models | universal models |
| θ | volumetric water content, $\text{m}^3 \text{m}^{-3}$ |
| θ_0 | parameter of the $\kappa(\theta)$ function; water content corresponding to the highest thermal diffusivity, $\text{m}^3 \text{m}^{-3}$ |
| κ | thermal diffusivity, $\text{m}^2 \text{s}^{-1}$ |
| κ_0 | parameter of the $\kappa(\theta)$ function; thermal diffusivity of dry soil, $\text{m}^2 \text{s}^{-1}$ |
| ρ_b | wet bulk density, kg m^{-3} |

Temporal variability of soil thermal diffusivity is related primarily to the natural temporal variability in soil moisture (Roxy, Sumithranand, & Renuka, 2014, 2010; Sugathan, Biju, & Renuka, 2014). Spatial variability may also be explained to some extent by the spatial variability of soil moisture, but it usually turns out that the fundamental cause is the spatial variability of soil texture, bulk density, and organic carbon (Arhangelskaya, 2004).

The necessity to estimate soil thermal properties from available data arises in various fields of biosystems and geosystems studies. Examples are assessments of the energy budget at the soil–air interface (Peters-Lidard, Blackburn, Liang, & Wood, 1998); assessments of the subsurface heat storage (Popp, Beyer, Dahmke, & Bauer, 2015); constructing the geothermal systems (Busby, 2016); and modelling coupled water and heat transfer in soils (Simunek, van Genuchten, & Šejna, 2016).

The existing models of soil thermal properties have been discussed by Barry-Macaulay, Bouazza, Wang, and Singh (2015). Most authors use data on soil texture, bulk density, organic

carbon, and soil moisture (Rozanski & Stefaniuk, 2016; Tian, Lu, Horton, & Ren, 2016). The modelling accuracy is rather low. For example, the determination coefficient (R^2) for the recently published de Vries-based model for soil thermal conductivity by Tian et al. (2016) was 0.79, which was better than 0.69 for the previous Farouki–de Vries model (Farouki, 1981, 1982).

Quite often only a few soil data are available to make necessary estimations, and so the objective of our research was to develop models which can work even with a minimum amount of input information.

When developing our models we followed the same hierarchical approach that was used in the computer program ROSETTA to estimate soil hydraulic parameters (Schaap, Leij, & van Genuchten, 2001): when the only soil information available is the name of textural class, then the soil thermal diffusivity vs. water content dependency is predicted based on this name only. If detailed data on soil texture are available, then the regression model is used with higher accuracy, and when data on bulk density and/or organic carbon are incorporated, the model estimates of soil hydraulic parameters become more precise.

The second approach we borrowed from soil hydrology was grouping soils (Pachepsky & Rawls, 1999). When applying this method, the whole training dataset is first used without any grouping. Next, soils are grouped by texture (or by any other predictors), and regression models are trained separately on each of the subsets. Such a grouping-based approach has been applied by Pachepsky and Park (2015) and gave good results when modelling saturated hydraulic conductivity of US soils.

2. Material and methods

2.1. Data sources

Models were developed from the measured $\kappa(\theta)$ curves, where κ is thermal diffusivity and θ is water content. Undisturbed soil cores were sampled with thin-walled steel cylinders in Suzdal region (56°23'N, 40°25'E), Moscow region (56°2'N, 37°10'E and 54°55'N, 37°34'E), Kamennaya Steppe (51°03'N, 40°43'E), and Adygea (44°50'N, 40°30'E). Sampling plots are marked in Fig. 1a. The soil cores sampled in Kamennaya Steppe were 70 mm in height and 50 mm in diameter; all other cores were 100 mm in height and 38 mm in diameter.

Experimental dependencies were obtained by the unsteady-state method (Abu-Hamdeh, 2003; Arhangelskaya, 2004; Parikh, Havens, & Scott, 1979). One junction of the differential copper-constantan thermocouple was inserted into the centre of the core, another junction was left outside. The soil core was covered and left overnight to equilibrate with the room temperature of 18–20 °C. Then it was immersed into the water bath with a constant temperature of 25 °C, and the voltage in the thermocouple loop was registered for 8–10 min. This voltage was proportional to temperature difference between the thermocouple junctions, that is, between the centre of the sample and the water bath. The rate of the voltage decline due to soil warming in the course of the experiment was proportional to soil thermal diffusivity.

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