Thermal conductivity modelling of terrestrial soil media—A comparative study

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Abstract

The paper describes prediction of thermal conductivity in terrestrial soil media. The model operates statistically by probability of occurrence for contacts between particular fractional compounds. It combines physical properties, specific to particular compounds, into one apparent conductance specific to the mixture. The concept of substituting grain compounds by hypothetical spheres is an essential tool to control porosity by the number of spheres, their radii and probability of contacts between them. The spheres are equal in radii. The spheres substitute compounds, regardless of the phase state. Control of particular phase states is possible by means of specific properties assigned to the spheres, at the input to the model. Performance of the model is successfully proved for many diverse terrestrial soil media in a wide range of bulk density, composition, water and water vapour content. Only the compounds of sand decline from the expected values and require introducing a correction to the thermal conductivity of sand grains. One possible explanation is that the thermal conductivity of sand is uncertain. Nevertheless, the model is useful and worth extending beyond terrestrial purposes.

Keywords: Thermal conductivity prediction; Statistical–physical model; Soil water; Soil porosity; Temperature

1. Introduction

Porous soil media are composed of solid, liquid and gaseous phases that are represented by different constituents depending on the environment. Thermal conductivity is an important factor influencing the surface-energy partitioning and energy flux in the porous media under terrestrial and extraterrestrial conditions. The thermal conductivity of the soil media is highly affected by texture, mineralogical composition and organic matter content that are inherent to the porous media, and by more variable factors including water content, temperature, and porosity, as well as by gas pressure and water vapour content (Steiner and Kömle, 1991; Tarnawski and Leong, 2000; Ochsner et al., 2001). Other works consider more rigorously the coexistence of CO, CO_2 and H_2O, in solid phase of ice with their gaseous phases (Espinasse et al., 1991; Shoshany et al., 2002). The effect of texture on the thermal conductivity was clearly demonstrated in laboratory experiments indicating that the addition of only a few percent of wax cement to organic granular materials (Seiferlin et al., 2003) or organic matter to mineral soil samples (Rovdan and Usowicz, 2002) causes significant change in the thermal conductivity. The effects of water and temperature on the thermal conductivity are interrelated. In general, the thermal conductivities of wet porous particle packed beds increase with increasing temperature in contrast to the behaviour of dry beds (Blumberg and Schlünder, 1995; Büssing and Bart, 1997). In wet beds this is a reflection of not only greater thermal conductivity of water but also of the strong temperature-dependent equivalent thermal conductivities arising from steam diffusion. In the case of porous water ice, a strong increase of the thermal conductivity was recorded at temperatures close to the sublimation temperature of water ice due to heat transport by pore-filling vapour. In general, an increase in initial moisture content leads to uniform...
moisture distribution, thus a uniform thermal conductivity (Singh and Chaudhary, 1995).

Volume fractions of porous media are significantly influenced by cementation or compaction and associated increase in density (Lipiec and Hatano, 2003). Cementation can be a very effective process to increase the thermal conductivity and thermal inertia of porous media, like soil (Usowicz et al., 1996; Guérif et al., 2001), dust and regolith (Seiferlin et al., 2003). This increase is ascribed to mostly greater contact between the primary particles. The effect of soil density on thermal conductivity was more pronounced at high (field capacity or greater) than at medium soil water contents (Horn, 1994; Usowicz et al., 1996). It was shown that aggregated soil, compared to disturbed soil, is characterized by greater heat flow irrespective of bulk density Türk et al. (1991). This effect is provided by the continuity of contact points between primary particles (conductance), improved by water-filled pores and enhanced by convection and diffusion of water and air.

Porous materials like mineral compositions and granular materials, porous water ice, or carbon dioxide ice are common constituents of planets and comets in the solar system (Gori and Corasaniti, 2004). Data from the Viking Pathfinder and Mars Global Surveyor missions imply that the outer crust of Mars contains significant amounts of andesites and basalts (Mc Sween et al., 1999) and therefore they may significantly affect the thermal conductivity.

Since a variety of porous media occurs under space conditions, a wider range of sample materials and compositions in relation to variable factors is advised to be included in thermal experiments. Gori and Corasaniti (2004) reported that thermal properties of the Martian regolith and megaregolith approximate those of soil analogues in either dry or frozen state and are suitable for model prediction of the thermal conductivity versus porosity and ice contents of Mars. Consistent estimates of extraterrestrial soil analogues thermal conductivity are useful in predicting these properties of porous materials under space conditions. Thermal conductivity is a subject of investigation of granular materials, aimed at understanding the nature of thermal evolution of a comet nucleus (e.g., Sirono and Yamamoto, 1997).

In this paper, we shall present a statistical–physical model and its performance in predicting the thermal conductivity of various porous terrestrial soil media. The presented model and available experience from soil physics on the Earth may deserve some notice in investigations of space bodies.

2. The model

Soil is assumed to be a homogeneous mixture of components. It is a composition of several or many fractions of component particles. Each component fraction is also known by the statistical size distribution of grains. The medium is understood to be homogeneous statistically that is in the scale of the entire unitary volume.

The purpose of the model is to assess the specific thermal conductivity of soil as determined by soil composition and external conditions. Particular component fractions are known by specific properties of the bulk material—mass density, thermal conductivity, and by the fraction in the total amount of the unitary volume. The specific properties and fractions cover dependence on temperature and pressure respecting other necessary conditions for the determination of phase state changes. The range of applicable external conditions is constrained by available property definition, but not by the model. The specific component properties are the input to the model. They determine the output thermal conductivity and are not constituents of the model.

The model was built for terrestrial applications and conditions but may be employed for other conditions if the specific component properties are definable. The model allows its employing in vacuum conditions.

Under steady-state conditions and in uniform and isotropic medium heat flux density \( q \) (W m\(^{-2}\)) is proportional to the temperature gradient \( \frac{\partial T}{\partial z} \) (K m\(^{-1}\)) along the direction of heat flow:

\[
q = -\lambda \frac{\partial T}{\partial z}.
\]

The proportionality coefficient \( \lambda \) (W m\(^{-1}\) K\(^{-1}\)), called the thermal conductivity, is a characteristic of the given medium.

The study employs the statistical–physical model of soil thermal conductivity proposed by Usowicz (Usowicz, 1991, 1992, 1995). The model is expressed in terms of heat resistance (Ohm’s law and Fourier’s law), two laws of Kirchhoff, and the polynomial distribution (Eadie et al., 1989). The volumetric unit of soil in the model (Fig. 1(a)) consists of solid particles, water and air, and is treated as a system made up of regular geometric figures, spheres, filling the volumetric unit by layers (Fig. 1(b)).

It is assumed that connections between layers of the spheres and the layer between neighbouring spheres will be represented by serial and parallel connections of thermal resistors, respectively (Fig. 1(c)). Comparison of resultant resistance of the system, with consideration of all possible configurations of particle connections together with a mean thermal resistance of given unit soil volume, allows estimating the thermal conductivity of soil \( \lambda \) (W m\(^{-1}\) K\(^{-1}\)) according to the equation (Usowicz, 1992)

\[
\lambda = \frac{4\pi u L}{\sum_{j=1}^{L} P(x_{ij})},
\]

where \( u \) is the number of parallel connections of soil particles treated as thermal resistors, \( L \) is the number of all possible combinations of particle configuration, \( x_{1}, x_{2}, \ldots \) \( x_{k} \) are numbers of particles of individual particles of a soil with thermal conductivity \( \lambda_{1}, \lambda_{2}, \ldots, \lambda_{k} \) and particle radii \( r_{1}, r_{2}, \ldots, r_{k} \), where \( \sum_{j=1}^{k} x_{ij} \lambda_{j} = u, j = 1, 2, \ldots, L, P(x_{ij}) \)—probability of occurrence of a given soil particle configuration calculated from the polynomial distribution.
The condition $\sum_{j=1}^{L} P(X = x_j) = 1$ must be fulfilled. The probability of selection of a given particle $f_i$, $i = s, l, g$, in a single sample is determined based on soil properties. The values of $f_s$, $f_l$, and $f_g$ are taken individually for composing fractions of minerals and organic matter as $f_s = 1 - \phi$, for liquids as $f_l = \theta_v$ and for air or gases as $-f_l = \phi - \theta_v$ inside the unitary volume, and within the assumed porosity $-\phi$ (m$^3$ m$^{-3}$).

The model was checked on many selected examples of soils with thermal conductivity known from experimental and literature data (Usowicz, 1992). It was determined that the number of the required parallel and serial connections of thermal resistors strongly depends on the water content and bulk density of the soil. The studied model was identified as a model which modifies the number of parallel connections of thermal resistors along with the change of the ratio of water content in the unit of soil volume to its porosity (Usowicz, 1992, 1995):

$$r_k = 0.036f_o + 0.044,$$

where $f_o$ (m$^3$ m$^{-3}$) denotes the content of organic matter in a unit of volume.

The stepwise transition of the value of $u$ as a function of soil saturation with water causes a respective step increase of calculated values of the thermal conductivity of soil. To avoid such transition, a procedure of intermediate determination of thermal conductivity in a range of soil saturation was proposed. The procedure is to determine thermal conductivity for two succeeding values: $u$ and $u + 1$ (Fig. 2) and then the values corresponding to the water content $\theta_v(u)$, $\theta_v(u+1)$. The linear equation given below determines thermal conductivity for the needed value of the water content of the medium $\theta_v$:

$$\lambda = \lambda(u) + \frac{\theta_v - \theta_v(u)}{\theta_v(u+1) - \theta_v(u)}(\lambda(u+1) - \lambda(u)).$$

Practically, the required experimental data are limited by a few routine physical measurements determining soil composition and calculation according to the model (Usowicz and Usowicz, 2004). The required reference data is specific to quartz ($\lambda_q$), other minerals ($\lambda_m$), organic matter ($\lambda_o$), water ($\lambda_w$) and air ($\lambda_a$) and then nearly all kinds of terrestrial soils are available for study of thermal conductivity by means of the model. Heat flow in a wet porous medium can be increased by the equivalent thermal conductivity of vapour when water evaporates from the warm region of the pore and moves due to gaseous diffusion and condenses on the cold region. This results in flow of latent heat of vapourization (Blumberg and Schlünder, 1995 and literature therein). This effect was included in the tested statistical–physical model by adding thermal conductivity of vapour to that of air (Appendix, Table 2).

Contents of main mineralogical components that are quartz and other minerals can be obtained by direct
measurements or by estimates based on fractional composition. In the case of the estimate one should analyse carefully the origin of a particular soil and choose soil fraction which represents mostly a given mineralogical component. It is accepted that quartz occurs mainly in the fraction 2–0.02 mm and other minerals in the fraction <0.02 mm (Usowicz and Usowicz, 2004). Based on the textural composition and the particle density of solid and organic matter, the volume fraction of quartz and other minerals, and organic matter was calculated.

The formulas employed to characterize soil components and procedure for calculating the thermal conductivity are given in Appendix (Table 2).

3. Data sets and statistical evaluation

We examined the accuracy of the physical–statistical model (Usowicz, 1992) using the measured data of the thermal conductivity from literature. The data were for three groups of terrestrial mineral soil media and two groups of organic soil media including peat and peat-sand mixtures.

The first group of mineral soil media included sand, clay and silty loam. A range of the thermal conductivity was obtained at different levels of water content and bulk density of the soils (Kersten, 1949, de Vries, 1963; Kossowski, 1977; Usowicz, 1992, 1995). The second group incorporated five mineral soils, that is Quincy, Ritzville, Walla Walla, Palouse, and Naff, having clay content of 1.5%, 5.5%, 9.4%, 12.4% and 23.4%, respectively (Mc Innes, 1981; Tarnawski and Leong, 2000). The content of sand was 95% in the Quincy soil and 20–30% in the remaining soils. The measured thermal conductivities were obtained at different levels of soil moisture and temperature. The third group consisted of four soils of sandy loam, clay loam, silt loam and silty clay loam texture, with organic matter ranging from 0.9% to 2.3%, from the work of Ochsner et al. (2001). The measurements of the thermal conductivity were taken over a range of volume fractions of Ochsner et al. (2001). The measurements of the thermal conductivity were taken at 4.4°C (Rovdan, 1997). The measurements of the thermal conductivity were taken at 10°C in the former and at 10°C in the latter at different moisture contents and bulk densities. The peat–sand mixtures consisted of a low-mire sedge peat (9% ash content and 25–30% decomposi-
tion degree) and quartz sand of 0.25–1 mm diameter. The proportions of the sand in the mixtures were 20%, 20–30%, 40–50%, 60–70%, 70–80%, 80–90% and 90–96% (Rovdan, 1997). The thermal conductivity of each mixture varied due to different moisture content (from air-dry to saturation state) and bulk density that resulted in a range of ratios of volumetric water content and porosity. The measurements were taken at 10°C.

To evaluate the performance of the statistical–physical model an error analysis was made, based on root mean square error (RMSE), maximum relative error (MRE) and determination coefficients ($R^2$) and linear regression coefficients. RMSE was calculated using the equation

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (f_{mi} - f_{ci})^2}{k}}$$

where $f_{mi}$ is the measured value, $f_{ci}$ is the calculated value, $k = n-1$ if $n < 30$ and $k = n$ if $n > 30$, $n$ is the number of data. The MRE was calculated from the equation:

$$\text{MRE} = \max_{i=1,2,...,n} \left\{ \left| \frac{f_{mi} - f_{ci}}{f_{mi}} \right| \times 100\% \right\}.$$  

Lesser values of RMSE and MRE indicate better agreement between the values estimated and measured, or lesser deviation.

4. Results

Evaluation of the first group of mineral soils (silt loam, clay and sand) gives the modelled and measured thermal conductivity values well agreed, with high $R^2$ ranging from 0.948 to 0.987 (Fig. 3). The RMSE of the conductivity ranged from 0.083 to 0.123 W m$^{-1}$ K$^{-1}$ and the MRE from 30.3% to 38.3%. The statistical evaluation indicates high accuracy in predicting thermal conductivity in the wide range of all mineral soils. Among the soils, the smallest RMSE and MRE are with respect to the sandy soil, indicating the least estimation deviation in predicting λ as compared to the other soils.

Evaluation of the second group of mineral soils (Quincy, Ritzville, Walla Walla, Palouse, and Naff) proved that the model also behaves well, with the determination coefficients of linear regression ranging from 0.894 to 0.968 (Fig. 4). The RMSE of the conductivity ranged from 0.06 to 0.091 W m$^{-1}$ K$^{-1}$ and the MRE from 28.4% to 83%.

The modelled values were notably higher than the measured values in the region of the largest thermal conductivities for the Quincy soil, which can be attributed to a much higher sand content (95%), having relatively high thermal conductivity, compared to other soils (20–30%) (Tarnawski and Leong, 2000). Among the soils, a relatively low thermal conductivity was exhibited by the Naff soil of low content of sand (20%). The Naff soil had the highest MRE and the lowest $R^2$.

With respect to the third group of mineral soils (sandy loam, clay loam, silt loam and silty clay loam) the evaluation indicated that the mean determination coefficient of linear regression was relatively high ($R^2 = 0.872$), but values from the statistical–physical model tended to underestimate the thermal conductivity in the region of low thermal conductivities (Fig. 5). The RMSE of the conductivity was 0.238 W m$^{-1}$ K$^{-1}$ and the MRE 58.3%.

The error analysis parameters (RMSE, MRE) and linear regression coefficients for all mineral soils indicate that the
accuracy of the statistical–physical model is satisfactory and comparable to that of the widely used model of de Vries (1963) (Usowicz, 1995; Ochsner et al., 2001).

Comparison of the measured thermal conductivity to the values predicted by the model for peat–soil is shown in Fig. 6 in above-zero and below-zero temperature ranges. The conductivity values at 4.4 and 10°C (Fig. 6(a, b)) are similar and considerably lower than those at −10°C (Fig. 6(c)).

The predicted and experimental data agree well in the entire range of temperature but the determination coefficient of linear regression is lower in the below-zero temperature range. This is an effect of changes in soil structure under freezing (Singh and Chaudhary, 1995). For the low-mire sedge of peat the model tends to underestimate (Fig. 6(b)) small conductivity values around 10°C, while high conductivity values around −10°C are overestimated (Fig. 6(c)). High values of conductivity at below-zero temperature are ascribed to the thermal conductivity of ice being greater than for liquid water in the above-zero temperature range. Heat conduction becomes improved under freezing though it may be moderated by changes in volume fractions of water and ice and decreasing soil bulk density. Gori and Corasaniti (2004) discussed the impact of the void space occupied by ice at the expense of atmospheric gas in the analogue Martian soil (olivine) on thermal conductivity. The authors showed that at the same ice volume content the thermal conductivity decreased with increase in the ice mass content, because the thermal conductivity of solid particle is higher than the ice value.

Comparison of the measured thermal conductivity to the values predicted by the model for peat-sand mixture soil is
shown in Fig. 7. Thermal conductivity increases with the fraction of sand having high conductivity. High correlation coefficient reflects good agreement between measured and predicted values (Table 1) and implies that the model can assist in predicting changes of the thermal conductivity of peat-mineral components.

5. Discussion

Several studies imply that the thermal properties of the space media depend on numerous compounds that occur in terrestrial soils (e.g., Gori and Corasaniti, 2004). Therefore, finding most appropriate terrestrial soil analogues is essential for gaining insight into the thermal conductivity of planets and other bodies of the solar system. Basalt (Moroz et al., 1991; Gunnlaugsson et al. 2002), olivine (Gori and Corasaniti, 2004), andesit and montmorillonite (Moroz et al., 1991), terrestrial frozen soils (Gori and Corasaniti, 2004) have been found to be possible Mars soil analogues.

Basalt consists of quartz in from 41% to 51%. The clay, silt loam and sand soils and peat–sand mixture used in our study contain similar or somewhat greater amounts of quartz. Moreover, the soils contain other components that occur in basalt, for example Al₂O₃, iron oxide and calcium oxide, magnesium oxide, and those that do not occur in basalt, for example organic matter. The thermal conductivities of the soils in dry state ranged from 0.04 W m⁻¹K⁻¹ for peat to 0.1–0.3 W m⁻¹K⁻¹ for mineral soils. Some of the soils, e.g., clay and silt loam, have conductivities of 0.1–0.15 W m⁻¹K⁻¹ that are very similar to that of olivine used as a Martian soil analogue (0.144 W m⁻¹K⁻¹) (Gori and Corasaniti, 2004). In general, soils of greater sand content in our study had greater thermal conductivities (approximately 0.3 W m⁻¹K⁻¹).

The results presented in the paper indicate high sensitivity of the statistical–physical model to various volume fractions of components that occur both in terrestrial and extraterrestrial soils. This supports the possibility of using this model with respect to space bodies with known content of main mineralogical components and porosity, highly influencing the thermal conductivity. Some knowledge on the main components of space bodies (e.g., basaltic soil rich in MgO and SO₃ on Mars) can be obtained from the previous space missions’ records (Morris et al., 2000), while required thermal conductivities of the components, from the physics handbook. When we know only the mineralogical composition, the statistical–physical model can simulate the thermal conductivity for hypothetical porosities that can be adjusted based on comparison...
of measured radiation temperature distribution and temperature simulated using hypothetic thermal conductivities.

At a given distribution of solid particles over a given volume, increase of the thermal conductivity is associated with increasing volume fraction of water and bulk density. Increase in volume fraction of water results in a greater number of water bridges between the solid particles. This is represented in our model by increased number of parallel-connected resistors. Increasing bulk density leads to a greater number of contact points and thus contact area between the solid particles. In other works (Squyres et al., 1985; Kossacki et al., 1994), the effect of contact area on the thermal conductivity is controlled by the Hertz factor being a ratio of contact area to total area. In the work by Shoshany et al. (2002), the corresponding reduction of the conductance value due to porosity does not require the Hertz factor or similar correction because the concept employs the hierarchical mesh of fractals, which implicitly implements porosity. In our model, the porosity is also implemented by increasing or decreasing compaction levels that are reflected in a greater probability of drawing by lot of solid phase or gaseous phase, respectively, and correspondingly in higher or lower thermal conductivities due to greater thermal conductivity of solid than gaseous phase. This model is able to react to pressure and water or water vapour content.

The results from the model reveal some discrepancy when the reference-measured values (Tsotsas and Martin, 1987; Büssing and Bart, 1997; Ould-Lahoucine et al., 2002) are contributed by sand quartz fractions. The sand and quartz particles, which have very different shapes with flat facets, strongly determine inter-particle contacts. That makes the sand particles diverging from the assumption of the spherical shape. We managed that by correcting the reference formulas determining input model parameters for sand particles sized 0.02–2 mm. The formulas on thermal conductivity for sand are given in Table 2 in the Appendix, and assume the reference value of 9 W m–1 K–1 while we employed some correction. The use of this thermal conductivity value for sizing 0.02–2 mm brings good agreement between the model and practically measured values for all types of mineral soils (as shown in Figs. 3–5), except for the peat-sand mixtures. For these peat-sand mixtures the values predicted by the model are a bit greater than experimental values in some range of soil moisture,

<table>
<thead>
<tr>
<th>Statistics</th>
<th>Mixed peat–sand</th>
<th>Peat (±10 °C)</th>
<th>Peat (–10 °C)</th>
<th>Peat (4.4 °C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE (W m–1 K–1)</td>
<td>0.083</td>
<td>0.036</td>
<td>0.281</td>
<td>0.022</td>
</tr>
<tr>
<td>MRE (%)</td>
<td>55.5</td>
<td>59.2</td>
<td>50.0</td>
<td>33.3</td>
</tr>
<tr>
<td>R2</td>
<td>0.937</td>
<td>0.975</td>
<td>0.895</td>
<td>0.9937</td>
</tr>
</tbody>
</table>

Table 1
Statistical summary comparison of measured and calculated thermal conductivity of mixed peat–sand and peat at above- and below-zero temperatures

<table>
<thead>
<tr>
<th>Reference</th>
<th>Expressions or values</th>
<th>Explanations</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Usowicz (1995)</td>
<td>λq = 9.103–0.028 T</td>
<td>Quartz</td>
<td>W m–1 K–1</td>
</tr>
<tr>
<td>de Vries (1963)</td>
<td>λm = 2.93</td>
<td>Minerals</td>
<td>W m–1 K–1</td>
</tr>
<tr>
<td>de Vries (1963)</td>
<td>λo = 0.251</td>
<td>Organic matter</td>
<td>W m–1 K–1</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>λw = 0.552 + 2.34 × 10–3 T–1.1 × 10–5 – T; λl = 2.2</td>
<td>Water or salt solution; ice</td>
<td>W m–1 K–1</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>λl = 0.0237 + 0.000064 T</td>
<td>Air</td>
<td>W m–1 K–1</td>
</tr>
<tr>
<td>de Vries (1963)</td>
<td>λapp = λl + λw</td>
<td>(See note)</td>
<td>—</td>
</tr>
<tr>
<td>de Vries (1963)</td>
<td>λ = exp((ρ Mw/ρwR(T + 273.15))</td>
<td>Relative humidity</td>
<td>—</td>
</tr>
<tr>
<td>de Vries (1963)</td>
<td>λs = LDs/d(ρd/dT)</td>
<td>Soil water pressure head — ψ</td>
<td>kPa</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>L = 490317–2259.4T</td>
<td>Molecular weight of water, Mw = 0.018</td>
<td>kg mol–1</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>λs = 0.0000229((T + 273.15)/273.15)1.75</td>
<td>Density of liquid water, ρw = 1.0</td>
<td>Mg m–3</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>λs = 21.7 × 10–8(101.325/P)((T + 273.15)/273.15)1.88</td>
<td>Universal gas constant, R = 8.3143</td>
<td>J mol–1</td>
</tr>
<tr>
<td>de Vries (1963)</td>
<td>v = P/(P – (hρwR(T + 273.15)/1000Mw))</td>
<td>(See note)</td>
<td>W m–1 K–1</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>v = P/(P – (hρwR(T + 273.15)/1000Mw))</td>
<td>Latent heat of vapourization</td>
<td>J kg–1</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>Ds = 21.7 × 10–8(101.325/P)((T + 273.15)/273.15)1.88</td>
<td>Diffusion coefficient for water vapour in air</td>
<td>m2 s–1</td>
</tr>
<tr>
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<td>Diffusion coefficient for water vapour in air</td>
<td>m2 s–1</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>ν = P/(P – (hρwR(T + 273.15)/1000Mw))</td>
<td>Mass flow factor</td>
<td>—</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>ν = P/(P – (hρwR(T + 273.15)/1000Mw))</td>
<td>Barometric pressure—P</td>
<td>kPa</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>ρs = 10–3 exp(19.819–4975.9(T + 273.15))</td>
<td>Saturated vapour density</td>
<td>kg m–3</td>
</tr>
<tr>
<td>Kimball et al. (1976)</td>
<td>dρ/dT = 49.57 9 ρs/(T – 273.15)</td>
<td>—</td>
<td>kg m–3 K–1</td>
</tr>
</tbody>
</table>

Note: For unsaturated soil, under high temperature gradient in the soil, the coefficient of thermal conductivity of air is replaced with the complex thermal conductivity (λapp) composed of the thermal conductivities of air λl and water vapour λl (Kimball and Jackson, 1975; Kimball et al., 1976). For salt-affected soils, under high gradient of salt concentration, the coefficient of thermal conductivity of water λw is replaced with the thermal conductivity coefficient of a given solution λq (Noborio and McInnes, 1993). The thermal conductivity of ice λs was used with respect to frozen soil.
with the regression coefficient of about 1.6 (Fig. 8). It was assumed that the overestimated thermal conductivity values of the mixtures from the model could be a result of too high value of the thermal conductivity used for the sand (0.25–1 mm) in this study. To overcome this constraint we reduced the thermal conductivity from 9 to 5 W m$^{-1}$ K$^{-1}$ in consecutive model iterations with steps of 0.5 W m$^{-1}$ K$^{-1}$. The model performance, as shown by $R^2$, remained the same in all iterations, whereas the regression coefficient approached values close to 1 at thermal conductivity 5.5 W m$^{-1}$ K$^{-1}$ (Fig. 8). Hence this value seems to be well fitted to real thermal conductivity of the sand in these mixtures. Büssing and Bart (1997) reported similar values of the thermal conductivity, that is 5.24 W m$^{-1}$ K$^{-1}$, for comparable sand particles (1 mm). This analysis suggests that modelling can be improved by more accurate evaluation of the thermal conductivity of sand used in the model. The data after Büssing and Bart (1997) indicate that thermal conductivity of the sand fraction in the range of sizing from 0.1 to 2 mm may vary from 2.7 up to 8.7 W m$^{-1}$ K$^{-1}$. Silt and clay particles are assigned in the formulas (Table 2 in the Appendix) to the thermal conductivity value of 2.93 W m$^{-1}$ K$^{-1}$ after de Vries (1963).

Another factor influencing thermal conductivity of porous media can be the shape of the solid particles. Real shape of silica-sand in modelling the thermal conductivity was simulated as a spheroid or ellipsoid depending on modelling approach (Ould-Lahoucine et al., 2002), and with respect to the model equation of Fricke (quoted by Ould-Lahoucine et al., 2002) it was well predicted when the spheroid was used. Assumption of the spherical shape of all particles in our model gave satisfactory predictions of the thermal conductivity with respect to different soil media.

Particle size distribution is frequently used to estimate mineralogical composition, mainly quartz and other minerals that have dominating effect on the thermal conductivity. This estimation is justifiable since most sand fractions consist of quartz, but different forms of quartz can be characterized by different thermal conductivities. However, silt and clay particles are considered as other minerals and one value of the thermal conductivity is used with respect to all of them in modelling approach (de Vries, 1963). Therefore, measurements of mineralogical composition of porous media could improve the accuracy of modelling.

6. Conclusions

A broad palette of the porous soil media, within a wide range of water content, bulk density and temperature, was analysed to examine the performance of the statistical–physical model in predicting thermal conductivity.

The model performs well in predicting the thermal conductivity of the soil media based on their mineralogical composition, water content, bulk density and temperature. The results indicate high sensitivity of the statistical–physical model to changes in volume fractions of components of terrestrial soils. Predictive capabilities of the model are limited when mineralogical composition is estimated from the fractional composition of the soil media. More accurate evaluation of the mineralogical composition of the media will result in better performance of the model. The model may be useful for searching for ways of assessing thermal conductivity of space bodies.

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Appendix. The formulas employed to characterize soil components and procedure for calculating the thermal conductivity

Procedure of calculating thermal conductivity in the model.

The example of calculation for sand (de Vries, 1963) at temperature of 5 °C is presented below. In the first step, the thermal conductivity for particular soil components was calculated (Table 2). The studied soil consists of four major components: quartz 8.963 W m$^{-1}$ K$^{-1}$, other minerals 2.93 W m$^{-1}$ K$^{-1}$, water 0.563 W m$^{-1}$ K$^{-1}$ and air 0.024 W m$^{-1}$ K$^{-1}$, which are used to compute the average thermal conductivity of the sand. The content of each fraction is treated as the probability in a single sample. We denote by $x_q$—quartz content, $x_m$—content of other minerals, $x_s$—content of the solid phase, $x_w$—content of

\[
y = 1.609x - 0.186
\]

\[
R^2 = 0.942
\]

\[
y = 0.966x + 0.056
\]

\[
R^2 = 0.937
\]
water, and \( x_a \)—content of air in volumetric units. The values of \( x_k \) and \( x_m \) were computed from the de Vries’ formula, taking into account the division of the solid phase. They are: \( x_k = 0.665, x_m = 0.004, x_a = 0.331 \text{ m}^3\text{ m}^{-3} \) and \( x_k = 0.606, x_k = 0.403, x_m = 0.394, x_a = 0.262 \text{ m}^3\text{ m}^{-3} \).

Let us substitute for \( f_1 = x_q, f_2 = x_m, f_3 = x_a, f_4 = x_k \) in Eq. (3). The following part of the Eq. (2) was denoted as \( a_j \): 

\[
a_j = \frac{1}{\Sigma_{i=1}^{4} q_i x_{qi} + \lambda_m x_{m} + \lambda_a x_{a} + \lambda_k x_{k}} \frac{1}{\lambda_k}.
\]

In this equation for each \( q_{ij}, m_{ij}, a_{ij}, k_{ij} \), the different number of each particle was considered, under the condition \( \Sigma_{i=1}^{4} x_{qi} = u, i = q, m, w, a; j = 1, ..., L \).

The value of \( r_k \) being 0.044 m was calculated from the Eq. (4) for radius of sphere. Number of parallel connections, \( u = 3 \), for the water content, \( x_w = 0.004 \text{ m}^3\text{ m}^{-3} \) was taken from Fig. 2. This number leads to a given combination of particles which has to be considered (Table 3). Table 3 presents also the values \( a_j \) and probability of occurrence of a given particle combination.

In the statistical–physical model, the number of parallel connections and associated thermal conductivity changes stepwise with a change of water content. To minimize the stepwise changes in the model, a smoothing procedure based on linear equation (Eq. (5)) was applied. The calculated thermal conductivity, with consideration of the procedure, for the water content of 0.004 m\(^3\) m\(^{-3}\) was 0.404 W m\(^{-1}\) K\(^{-1}\) that was closer to the measured value (0.38 W m\(^{-1}\) K\(^{-1}\)) than the calculated value without consideration of the smoothing procedure (0.305 W m\(^{-1}\) K\(^{-1}\)). An example software implementation of the procedure is available from the co-author Usowicz@demeter.ipan.pl.

### Table 3

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\( J \)—index, \( q \)—quartz, \( m \)—other minerals, \( w \)—water, \( a \)—air.

### References


