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Modeling Soil Heat Flux in R

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ABSTRACT

Knowing of soil heat flow properties of a crop field inform the farmer about temperature conditions of seeds germination. Soil heat flow is either measured or modeled. In our study we rely on the procedure developed by Sang-Ok Chung and Robert Horton (1987). With the R language version of their heat flux model we studied on data collected by Gábor Szász (director of the Agro-meteorological Observatory of Debrecen in May 2001.). Soil temperature data were collected in 5, 25 and 50 cm depths in 15 minute intervals from a loam texture chernozem soil covered with short grass. The upper boundary layer at 5 cm and the lower boundary at 50 cm soil temperature data contain 2976 time periods. Using the R programmed heat flux model the 25 cm depth soil temperatures were simulated and compared to the measured ones. Since the simulated and measured soil temperatures differed significantly we assumed necessity of coupling heat and moisture flux for describing time change of soil temperate.

1. Introduction

Information of the heat flow is very important in research of agricultural soils because seed germination, tillering of cereal crops, plant mineral supplementation, plant root growth and respiration, soil microbe life, decomposition of plant parts, soil structure formation, moisture (liquid and vapor) transportation in soil, and soil decay depend on the temperature of the soil.

Soil heat flow today is either measured or modeled (Sándor and Fodor 2012a, Sándor and Fodor 2012b, Sándor, et al., 2013). The first computer models of heat flow in the soil were constructed in the 1970ies (Hanks et al., 1971). In our publication we rely on the procedure developed by Sang-Ok Chung and Robert Horton (1987). The original program was published in FORTRAN language in September 1986 (Hanks and Ritchie, 1991). Although this program incorporates a water flow model too, the procedure description suggests that when the temperature of the intermediate soil layers is to be modeled, this water flow model can be ignored in case measurement data on the temperature of the upper and lower boundary soil layers are available. We translated the original heat flow model into R language (R Core Team, 2013), and examined the model's correctness.

2. Material and method

In the model we used the following thermodynamic terminology (specific heat capacity, density, volumetric heat capacity) and their values (Table 1).

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Table 1. Thermodynamic parameters of certain soil contained materials

Materials	Specific heat capacity ($Jg^{-1}°C^{-1}$)	Density (gcm^{-3})	Volumetric heat capacity ($Jcm^{-3}°C^{-1}$)
Water	4.2	1	4.2
Air	1	0.0012	0.0012
Sand	0.84	2.5952	2.18
Clay	0.92	2.7173	2.5
Mould	1.7	1.6	2.72
Ice	2.1	0.8952	1.88

Under normal conditions, the volumetric heat capacity of the soil is determined by the compositional proportion of its components of which solid components and moisture content are the most decisive.

2.1. Volumetric heat capacity of wet soils

$$C_V = \rho_m 0.84 Jg^{-1}°C^{-1} + N_V 4.2 Jcm^{-3}°C^{-1} + L_V 0.0012 Jcm^{-3}°C^{-1} \quad (1)$$

where:

C_V : volumetric heat capacity (($Jcm^{-3}°C^{-1}$))

ρ_m : bulk density of the soil (gcm^{-3})

N_V : volumetric water content (cm^3cm^{-3})

L_V : volumetric air content (cm^3cm^{-3})

or if air is disregarded

$$C_V = \rho_m \left(0.84 Jg^{-1}°C^{-1} + N_m 4.2 Jg^{-1}°C^{-1}\right) \quad (2)$$

where:

N_m : water content (gg^{-1}).

In view of the above, the Q_q measure of exchange heat in „V" volume is determined by T_1 initial and T_2 final temperatures.

$$Q_q = C_V V (T_2 - T_1) = C_V V \Delta T \quad (3)$$

Volumetric heat capacity is the mathematical product of specific heat capacity and density. For calculating volumetric heat capacity under normal soil conditions, the bulk density of the soil (ρ_m) instead of soil density (i.e. ρ, which expresses the density of the solid parts) is to be considered.

As seen in Figure 1, volumetric heat capacity of the soil grows linearly with the growth of soil moisture content. This value is higher in compact soils (e.g. stubble) than in loose soils (e.g. plow land soil).

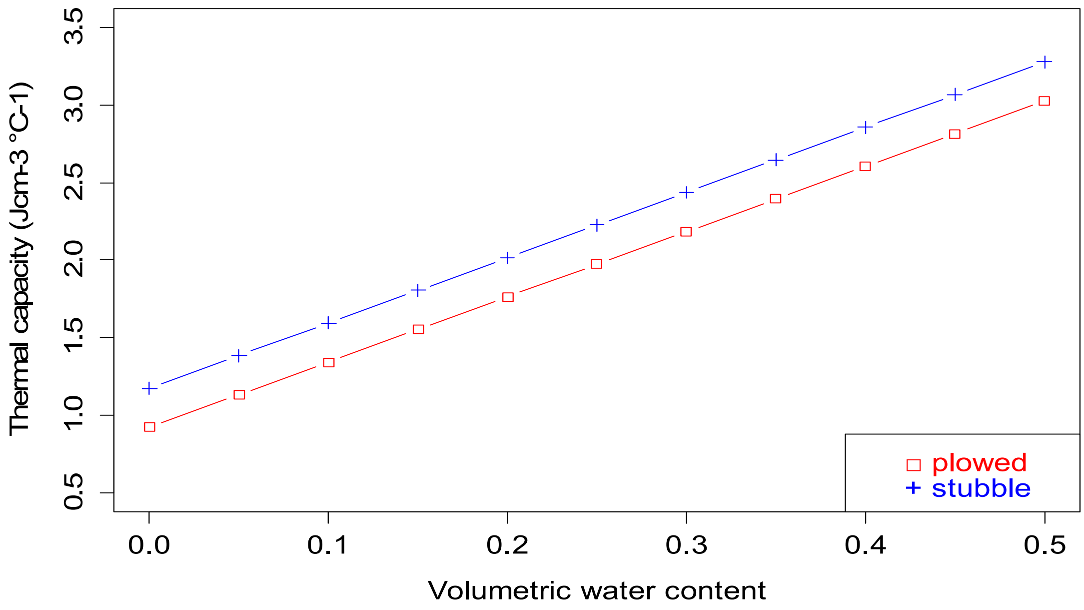

Figure 1. Soil volumetric heat capacity in function of soil moisture content

Soil heat transfer means heat transmission from molecule to molecule with material parts remaining in place.

$$Q_q = -K_q At \frac{\Delta T}{\Delta z} \quad (4)$$

where:
Q_q : quantity of heat (J)
K_q : thermal conductivity (W m^{-1} °C^{-1})
A : surface (m^2)
t : time (s)
ΔT : temperature difference (°C)
Δz : soil layer thickness (m)

The thermal diffusivity of the soil is the ratio of thermal conductivity and volumetric heat capacity, as used in the model.

2.2. Modeling heat flux

Modeling the thermal regime of the soil has two major phases:

1. Energy distribution on the soil surface.
2. Modeling heat distribution and flux in the soil profile.

In this publication we are dealing with the later only.

Heat fluxes in the soil can be described by the following equation:

$$G = -K_q \frac{\Delta T}{\Delta z} \quad (5)$$

where:
G : heat flux (positive, downward) (MJ m^{-2} d^{-1})
K_q : thermal conductivity (W m^{-1} °C^{-1})
ΔT : difference of temperature (°C)
Δz : soil layer thickness (m)

Variable G is determined by the unknown soil surface temperature. To be able to calculate soil surface temperature, the right side of the equation has to be expressed numerically. For this Chung and Horton (1987) recommend the following formula:

$$G = -K_q \left(\frac{T_2 - T_s}{\Delta z} \right) + (T_s - T_1) C \frac{\Delta z}{2 \Delta t} \tag{6}$$

where:
G : soil heat flux (positive, downward) (MJ m^{-2} d^{-1})
K_q : thermal conductivity (W m^{-1} $°C^{-1}$)
T_s : soil surface temperature at the given time period (°C)
T_1 : soil surface temperature at the previous time period (°C)
T_2 : temperature of the second soil layer at the antecedent time period (°C)
C : volumetric heat capacity (J m^{-3} $°C^{-1}$)
Δz : soil layer thickness (m)
Δt : time increment (s)

The temperature of the soil surface can be numerically calculated for every time step. For the calculation of the energy balance, James et al (1977) recommended to use the method of algorithmic root-finding.

2.3. Heat flux model in R

The model to be described here represents one dimensional vertical heat flux. The analytical description is as follows:

$$C \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(K_q \frac{\partial T}{\partial z} \right) \tag{7}$$

where:
C : volumetric heat capacity (J m^{-3} $°C^{-1}$)
T : soil temperature (°C)
K_q : thermal conductivity (W m^{-1} $°C^{-1}$)
∂t : time increment (s)
∂z : soil layer thickness (m)

The thermal conductivity of the soil (K_q), however, is not a constant value; it is greatly influenced by the water content of the soil which, in addition, varies by depth and time.

For the estimation of the volumetric heat capacity of the soil we used the 2. equation, whereas McInnes (1981) algorithm was applied for the definition of thermal conductivity. According to the algorithm, thermal conductivity is determined by the bulk density, by the sand content, by the clay content and by the water content of the soil.

To solve the tridiagonal matrix, in their original publication the authors used the Thomas algorithm which is an algorithm applicable to all programming languages, anyway. In our research and calculations we used this algorithm in *R language.* It proved to work perfectly. The algorithm is as follows:

```
thomas=function(w, b){
  n=nrow(w)
for (i in 2:n){
    ff = w[i, 1] / w[i - 1, 2]
  w[i, 2] = w[i, 2] - ff * w[i - 1, 3]
  w[i, 1] = ff
}

#   This is the elimination, the b is the input vector in the right
side, this is the solution vector also.
for (i in 2:n){
```

```
    b[i] = b[i] - w[i, 1] * b[i - 1]
}
# 'Substitution
  b[n] = b[n] / w[n, 2]
for (i in 2:n){
  j = n - i + 1
  b[j] = (b[j] - w[j, 3] * b[j + 1]) / w[j, 2]
}
return(b)
}
```

In an R environment, however, it makes no sense to use the Thomas algorithm, because the built-in linear algebraic equation solving algorithm (solve( )) produces the very same result, once the coefficient matrix is expressed in the form of real tridiagonal matrix.

The testing of the model was carried out on the basis of data of May 2001 acquired from the Agro-meteorological Observatory of Debrecen (director: Gábor Szász). In the Observatory the measurements are made in a soil with short cut grass at three depths (5, 25 and 50 cm) in 15 minute intervals by an automatic measurement and data collecting device. We had soil temperature data compiled from the three soil layers at a total of 2 976 time periods (31 days * 24 hours/day * 4/hours). We used temperatures at the upper boundary layer of 5 cm and the lower boundary layer of 50 cm depth layer. The temperature of the 25 cm depth layer was modeled and compared with the actually measured values.

The soil texture is sandy loam with bulk density of 1.4 gcm^{-3}, 60% sand, 20% clay, and 20% silt content for each soil layer. Based on this, the thermal diffusivity of the layers by McInnes (1981) was found to be 8.7E^{-7} m^{2}s^{-1}.

3. Result

Modeled and measured data are demonstrated in Figure 2.

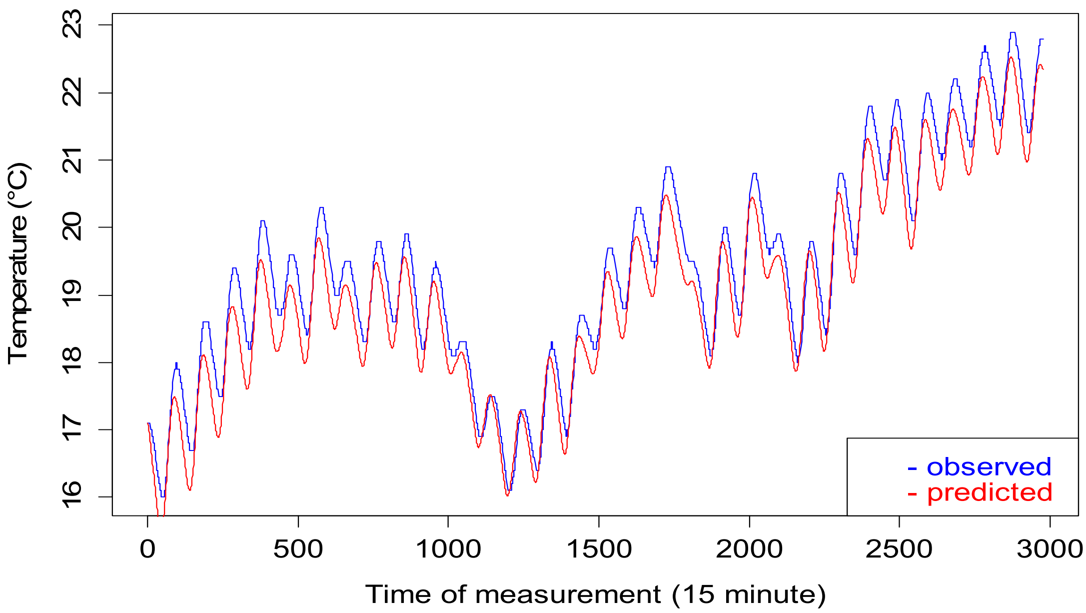

Figure 2. Modeled and measured temperature data of 25 cm depth layer. Debrecen, May 2001; measurements instrumented at 15 minute intervals

The modeled data fit for the measured data well, but the modeled data often underestimate the actual values.

3.1. Correctness of the model

The correctness of the model was defined by the simple statistical analysis of the residuals between measured and modeled temperatures

Deterministic models are considered to be correct, if the residuals between measured and modeled values are

1. Independent;
2. Have normal distribution zero expected value;
3. Are homoscedastic (variances are all uniform).

Figure 3 shows the errors against time. There is a type of fluctuation seen, which is likely to originate from the alterations of the soil humidity levels that keep altering the thermal diffusivity of the soil layers. Since there was no humidity measurement data available, the model was run with a deemed value of 20 vol. % humidity.

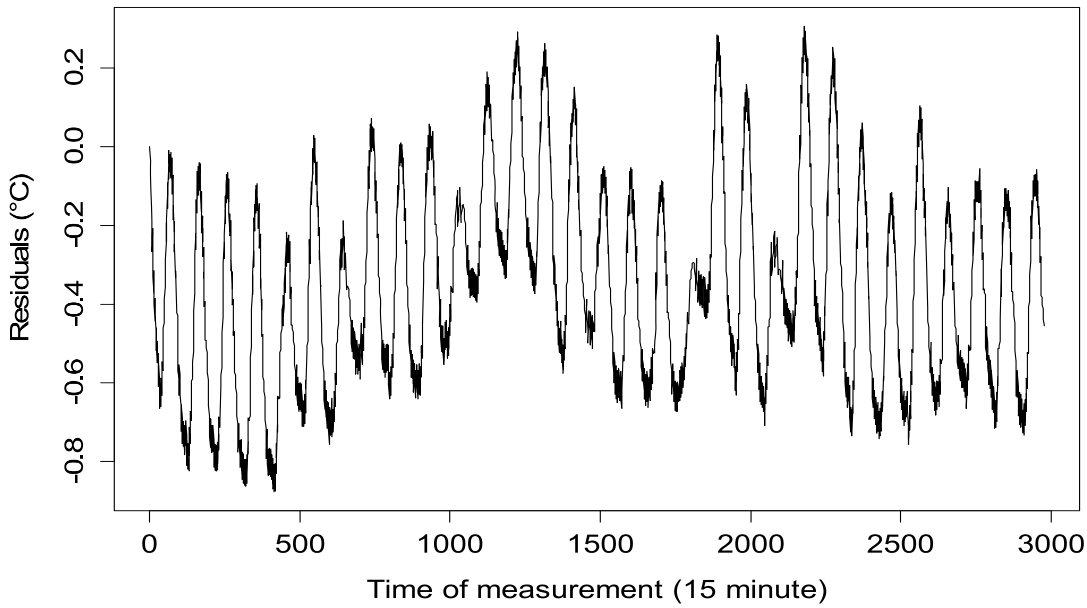

Figure 3. Differences between modeled and measured temperature data of 25 cm depth layer. Debrecen, May 2001; measurements instrumented at 15 minute intervals

The measure of the residuals keeps altering against time, which indicates that the first condition has not been fully met. In addition, there is a daily regular fluctuation pattern observed, which shows a sine rhythm repetition day by day (Figure 4). As a result, during the measured period there were 31 peek points identified.

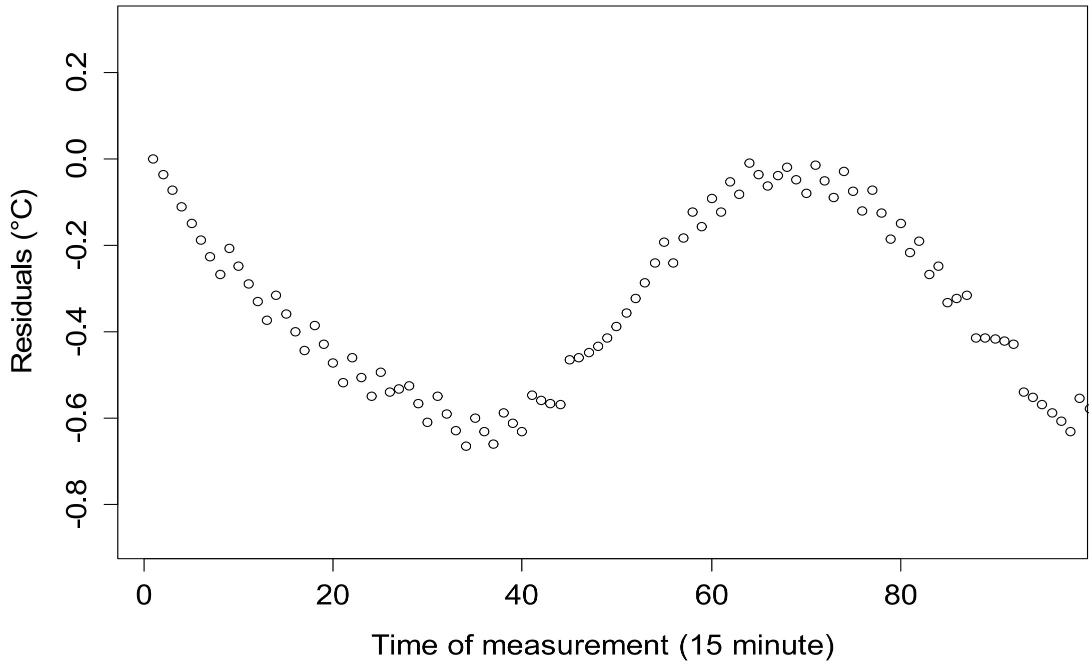

Figure 4. Errors of modeled temperature data of 25 cm soil depth layer.
Debrecen, 1st of May, 2001; measurements instrumented at 15 minute intervals

Axis x in Figure 4 shows 15 minute intervals of measurements; Zero and 40 indicate midnight and 10 am, respectively. The graph reveals the errors of the estimations: the estimated values do not correspond to the measured values in general, in particular the differences between them tend to increase in the time interval between midnight and 10 am, and decrease between 10 am and 16 pm. This is a systematic fluctuation of values.

The histogram of the residuals is demonstrated by Figure 5. Majority of the distribution values fall in the negative field, which is in tune with the above said.

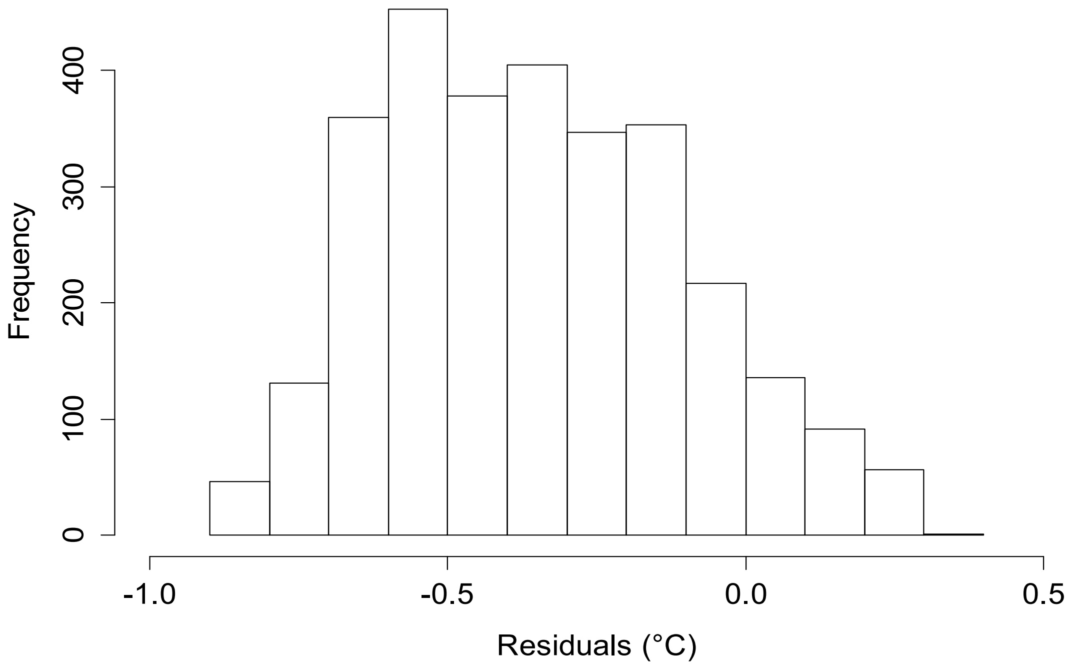

Figure 5. Errors of modeled temperature data of 25 cm depth layer. Debrecen, 1st May, 2001

Single-sample Kolmogorov-Smirnov test shows a non-normal, definitely asymmetric distribution of the residual. The expected value of the residuals is -0.35 °C.

To eliminate these errors, we modified the mode of estimating the average thermal diffusivity, which in the original model was a simple algebraic average. In their publication Horton and Chung notice that geometric methods may be more apt to estimate average thermal diffusivity between two layers, yet, they actually do not apply this method in their model. We tested the geometric estimation method, but it was not found better than the simple algebraic one; it kept having the same errors.

The homoscedasticity of the model is shown in Figure 3. The measure of the fluctuation of the residuals is not a constant value, it is time-dependent.

4. Summary

In our paper we examined the Chung and Horton (1987) model of heat flow and, following the recommendation of the authors, we run it with the exclusion of the water flow model. The original program developed in FORTRAN language was translated into R language and was modeled in an R environment. The temperature of the intermediate layer of a three-layer soil profile was estimated on the basis of the known temperature values of the upper and lower layers. The correctness of the model was tested with statistical methods. The heat flow model ignoring the water flow model produced the following results:

- The differences between observed and predicted temperature values depend on time (changes of soil moisture content), and show a regular daily sine rhythm. The daily rhythm is likely to be caused by the solar elevation and by the movement of moisture in the form of vapor.
- The residuals averages do not show a normal distribution with zero expected value; instead, they show a heavy asymmetry to the left direction. Hence, the instances of underestimation are much more frequent.
- The measure of the fluctuation of the residuals is not constant, either; it is also time-dependent.
- When estimating average thermal diffusivity, no difference between algebraic and geometric averages was found.

The program translated into R language turned out to be much shorter. The Thomas algorithm can be ignored if the coefficient matrix is expressed in the real tridiagonal form; in this case the R solve() function can be used.

Our final conclusion is that because of the strong correlation between water flow and soil temperature, it is essential to make simultaneous estimations of them both when modeling soil temperature.

This model can be used for estimating the temperature of the soil when the installed, vertically placed thermometers get out of order and it is necessary to replace the missing data. In this case the measured data can be used as boundary conditions and the middle temperature can be estimated with less error than any calculated mean.

By this model substituting of missing or erroneously measured data is also possible.

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