Full Length Research Paper

Application of numerical method in the estimation of soil thermal diffusivity and soil temperature prediction under different textures and moisture contents

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Numerical solution of heat conduction equation was used to estimate the soil thermal diffusivity (α) under different texture and moisture contents. The estimated value of was applied to soil temperature prediction at several depths and times. The results showed that the values of α at the beginning increased with increased moisture up to a critical point and then decreased. The maximum values for α occurred at 15 and 10% moisture contents for silty clay and sandy soils, respectively. Results of soil temperature prediction showed both overestimated and underestimated trends. The range of errors in most cases was ±1°C.

Key words: Thermal diffusivity, numerical method, moisture, soil temperature, texture.

INTRODUCTION

Soil temperature is a factor of primary importance in determining the rates and directions of soil physical properties and strongly influences its biological processes, such as seed germination, seedling emergence and growth, root development and microbial activity (Hillel, 2004). Soil temperature is often needed to model nitrogen transformation, thermal and biological degradation of land-applied chemicals (Ewa et al., 1990). Soil thermal properties including thermal conductivity, heat capacity and thermal diffusivity play an important role in the surface-energy partitioning and resulting temperature distribution (De, 1987; Horton and Chung, 1991; Noborio et al., 1996) and consequently form the soil and near ground atmosphere microclimate for plant growth (Heilman et al., 1996; MCINNES et al., 1996; Lipiec et al., 2007).

The soil diffusivity is determined by dividing its thermal conductivity by heat capacity and this is considered as the most important thermal characteristics of the soil which indicates the gradient of its warmth due to a unit change in its temperature. This parameter shows the ability of the soil in conducting the heat from a given point to another. Several methods are available to determine soil thermal diffusivity from observed temperature variations. Most of these methods are based on solutions of the one-dimensional heat conduction equation with constant diffusivity (Van Wijk, 1963; Nerpin and Chudnovskii, 1967; Wierenga et al., 1969; Singh and Sinha, 1977; Asrar and Kanemasu, 1983) and thus apply to uniform soils only.

In the absence of local heat sources or sinks, the equation that describes conductive heat transfer in a one-dimensional isotropic medium is:

$$C\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}(k\frac{\partial T}{\partial z}) \tag{1}$$

Where T = temperature (°C), t = time (s), z = depth (m) C = volumetric heat capacity (J/m^3. °C) and k = thermal conductivity (W/m. °C).

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Assuming C and k are independent of depth and time, Equation (1) then becomes:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial z^2}$$ (2)

Where α is the thermal diffusivity (m^2/ s), which is equal to k/C.

In general, the conditions for using Equation (2) include independence of α with respect to depth and time, one-dimensional heat flux and non-existence of any sources and sinks of heat within the soil. To make the α independent with depth and time, it is necessary that the soil profile remains homogeneous with respect to all parameters influencing C and k in the given time interval. The most influencing factors among these are mineral composition of soil, bulk density, air and moisture content of the soil (Hillel, 2004), where the moisture content is considered as the most important (Bachmann et al., 2001; Lipiec et al., 2007). For estimation of soil thermal diffusivity using Equation (2), several methods have been developed. Horton and Wierenga (1983) have tested 6 methods including: Arctangent equation, logarithmic equation, harmonic equation, numerical method, amplitude equation and phase equation and concluded that harmonic equation and numerical methods provided the most accurate results among all.

Application of the numerical method has the advantage of no corrections are needed for derivations from periodicity of the temperature wave of the upper soil boundary (Wierenga et al., 1969). 2 types of models were developed for soil temperature prediction (Bocock et al., 1977; Gupta et al., 1981; Parton, 1984) and included: (1) those based on the statistical relationship between soil temperature at different depths and climatological and soil variables and (2) those based on the physical principles of heat flow in soils. The latter model needs inputs of soil thermal characteristics, initial and boundary temperatures (Ewa et al., 1990).

In the present research, the soil thermal diffusivity (α) was estimated for 2 soil textures and 5 different moisture contents, using the numerical solution of Equation (2). Then, with specific initial and boundary conditions, the calculated optimum value of α for each case was applied in Equation (2) and soil temperatures at several depths and times were predicted. Comparing the predicted and observed temperatures, the performance of numerical method was evaluated.

MATERIALS AND METHODS

Laboratory measurements

For the experimental part of the work, a physical model, a chamber with dimensions of 500 × 500 × 800 mm, was made and its walls and bottom were carefully insulated using layers of plasto-foam sheets with a thickness of 100 mm. To test 2 textures of soil at the same time, the chamber was divided into 2 equal parts using the same insulating material as before. This condition satisfied the requirements for a one dimensional heat flow from the top surface to the bottom of the chamber. Then, the 2 parts of the chamber were filled with 2 soils with different textures namely; silty clay and sandy. The grain size distribution curves of the 2 soil types are depicted in Figures 1a and b.

To assure uniformity of the soil density in the chamber, the samples were placed in layers having 10 mm thickness and uniform compaction was applied by given numbers of tamping using a flat metal weight. For measurement of the temperature at different depths, special heat sensors were placed at the depths of 50, 110, 170, 250, 350, and 500 mm as well as at the top surface of the soils. The increasing distance between the sensors by depth, was due to higher temperature gradient at the upper part of the chambers. The sensors employed were SMT-160 - 30 and the maximum intrinsic error in the range of -30 to 100°C was ±0.7°C. The sensors were connected to a computer using an analog to digital converter system, where soil temperatures were recorded continuously at 1 min intervals. The data measurement for each case lasted for 24 h.

To eliminate evaporation from the top surface of the soil, it was covered by a plastic sheet. To control and change the temperature at the surface, a special cooling generating system capable of maintaining a constant temperature between +2 and +18°C was installed. A set of measured data in a time period of 12 h was used to calculate the optimum value of soil thermal diffusivity and another set in 12 h time period was employed to evaluate the model. All measurements were applied to 2 mentioned soil textures and gravimetric soil moisture contents of 0, 5, 10, 15, 20%, separately. These gravimetric moisture contents were prepared at the beginning of every experiment and immediately were transferred to the chamber.

Numerical calculations

The finite difference is considered as the most applicable method for numerical solution of the heat conduction equation in soils which is based on replacing partial derivatives by finite difference approximation and expanding by Taylor series (Gerald and Wheatley, 1989). To be able to solve the heat conduction equation, it was necessary to assume initial and boundary conditions from the beginning. The initial condition in the experimental model included the soil temperature at different depth at the beginning (t = 0) and the boundary conditions were specified by the known temperature or its gradient at the boundaries of the soil chambers for t > 0. For approximation of partial derivatives using finite differences, different algorithms may be used. In the present research, the Crank-Nicolson method which has a high degree of accuracy was employed. Using the above method, Equation (2) can be described as:

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^{n+1/2} - 2T_i^{n+1/2} + T_{i-1}^{n+1/2}}{(\Delta z)^2}$$ (3)

With $T_{i+1}^{n+1/2} = \frac{T_{i+1}^{n+1} + T_{i+1}^n}{2}$ and $T_i^{n+1/2} = \frac{T_i^{n+1} + T_i^n}{2}$.

Taking $d = \alpha \frac{\Delta t}{(\Delta z)^2}$, equation (3) can be rewritten as:

$$(1+d)T_i^{n+1} = \frac{d}{2} T_{i-1}^{n+1} + \frac{d}{2} T_{i+1}^{n+1} + \frac{d}{2} T_{i-1}^n + \frac{d}{2} T_{i+1}^n + (1-d)T_i^n$$ (4)
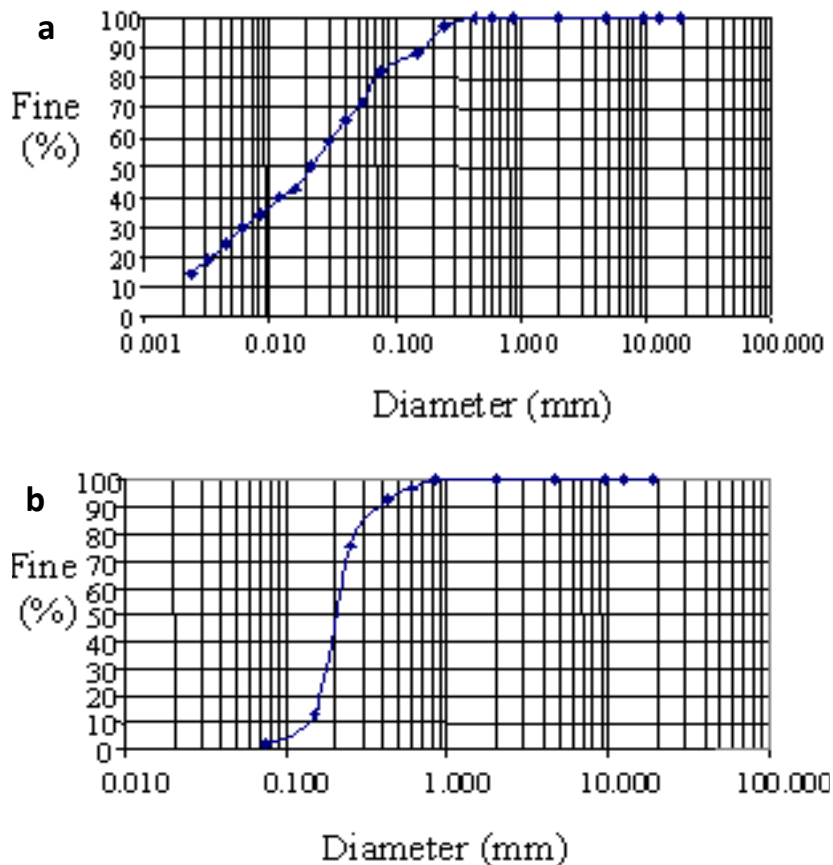
Figure 1a. Gradation curve of sandy soil, b. Gradation curve of silty-clay soil.

Where, n and i are the time and spatial intervals, respectively. One of the main advantages of the Crank-Nicolson method is its stability for all values of Δt and Δz.

However, the smaller the intervals, the greater will be the accuracy of the solution (Gerald and Wheatley, 1989). For numerical solution of Equation (4), time intervals of 1 s ($\Delta t = 1$ s) and spatial intervals of 1 cm ($\Delta z = 1$ cm) were employed.

Considering the fact that for computing a new temperature T_i^{n+1} in Equation (4), in addition to the known temperatures in the previous step, the temperature of the adjacent points at the same time interval, which are unknown were also employed. Thus, for each time interval a set of simultaneous equations will be made. These set of simultaneous equations can be solved using different methods. In the present research the Tree Diagonal Matrix Algorithm (TDMA) method was employed.

Determination of soil thermal diffusivity

If value of α is known, the above procedure can be employed to predict the soil temperature at any intermediate depth. In cases where α is unknown but the initial and boundary conditions are known and soil temperatures at different points and times have been measured, the optimum value of α can be determined using a trial and error technique. The approach is based on solving Equation (4) iteratively by changing α and determining the α value based on which the calculated values of temperature best

match observations. In the present work, the criterion used for choosing α was minimizing the root mean square error (RMSE) of the calculated (C_i) against measured (M_i) temperature:

$$RMSE = \sqrt{\frac{\sum(C_i - M_i)^2}{n}} \tag{5}$$

RMSE is a suitable criterion for the evaluation of a theoretical model, but it cannot provide any information on under-estimation or over-estimation of the results. For this purpose, the mean bias error (MBE) which is determined from the following relation can be employed:

$$MBE = \frac{\sum(C_i - M_i)}{n} \tag{6}$$

In Equations 5 and 6, C_i and M_i are the ith calculated and measured values and n indicates the number of data pairs.

As it was mentioned before, using half of the measured soil temperatures data set in a time period of 12 h, the optimum value of α was determined using numerical solution of Equation (2). The same procedure was employed for 2 mentioned soil textures and 5 different soil moisture contents. Then, by inserting the optimized value of α in Equation (2) for each case and considering the initial and boundary conditions from other 12 h measured data set, the soil temperatures for time and spatial intervals of $\Delta t = 1$ s and

Table 1. Values of α, RMSE and MBE for different soil moisture contents and textures.

Soil type	Moisture content (%)	m^2/s ($\alpha \times 10^{-4}$)	RMSE (°C)	MBE (°C)
Silty clay	0	0.0012	0.66	+0.54
	5	0.003	0.62	+0.52
	10	0.0058	0.71	+0.62
	15	0.0096	0.32	+0.27
	20	0.0084	0.53	+0.15
Sand	0	0.0014	0.68	+0.56
	5	0.0066	0.54	+0.47
	10	0.013	0.72	+0.53
	15	0.012	0.32	+0.27
	20	0.011	0.78	+0.61

Δz = 10 mm were predicted. Finally, accuracy of the numerical model was evaluated by calculating the difference between calculated and measured values for different cases.

RESULTS

Estimation of α value

The results of the application of numerical method for the determination of α in soils having different textures and moisture contents are given in Table 1. As it can be seen in the table, by increasing moisture content, the values of α for both silty clay and sandy soils were increased up to a certain point and then decreased. For all moisture contents, values of α in sandy soil was higher than those in silty clay. In dry condition (zero percent moisture content), the difference between α values for the 2 soils was negligible but by increasing soil moisture content, the difference became considerably higher. The maximum value for α was 0.0096 × 10^{-4} and 0.014 × 10^{-4} m^2/s for silty clay and sandy soils, respectively. The rate of variation of α due to the increase in moisture content was higher in sandy soil than silty clay. For example, by increasing moisture content from zero to 5%, the α value for silty clay increased from 0.0012 × 10^{-4} - 0.003 × 10^{-4} m^2/s, while for sandy soil it changed from 0.0014 × 10^{-4} - 0.0066 × 10^{-4} m^2/s.

Also, the moisture content at which α had the highest value was different for the 2 soil textures. This moisture content was 15 and 10% for silty clay and sandy soils, respectively. The estimation of α values was accompanied with some errors. Table 1 shows the RMSE and MBE values for each soil texture and moisture content. According to Table 1, RMSE values for different moisture contents in silty clay and sandy soil varied between 0.32 - 0.71°C and 0.32 - 0.78°C, respectively. The MBE values for the 2 soils varied between 0.15 to 0.52°C and 0.27 to 0.61°C, respectively. As shown in Table 1, the MBE values were all positive, which indicates that the overall trend of model most likely overestimated the results.
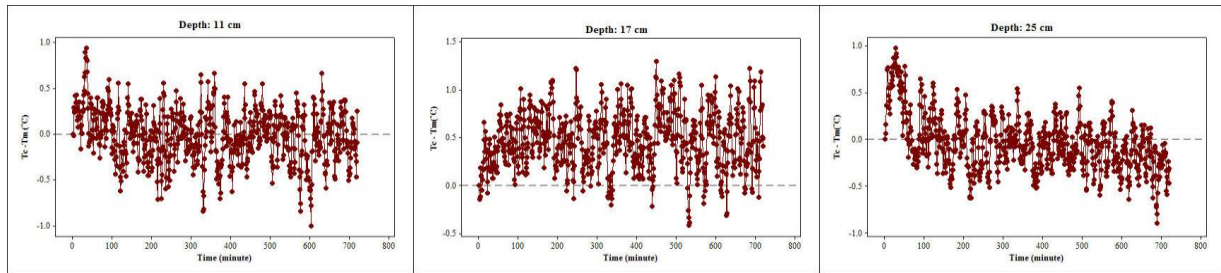
Soil temperature predictions

Figures 2a - e and 3a - e show the differences between measured and predicted soil temperatures and time at 110, 170 and 250 mm depths for all 2 soil textures and 5 moisture contents, separately. As shown in the figures, the predicted soil temperatures in some cases were higher and in some cases were lesser than the measured values. On the other hand, the results of finite difference model in some cases were overestimated and in the others were underestimated. But in general, the cases with overestimated results were most likely higher. The range of the difference between predicted and measured values in most cases was between -1 and +1°C. Also, in most of the cases, a clear trend in the difference between predicted and measured values with increased time during the time period of 12 h could not be observed.

DISCUSSION

As it was expressed above by increasing moisture content, the values of α for both texture soils were increased up to a certain point and then decreased. The main reason for this phenomenon was due to the nature of the variables in relation to defining soil thermal diffusivity (α) which is equal to *k/C,* where *k* is the thermal conductivity and *C* is the heat capacity of the soil. Based on the results of previous researches, increasing moisture content would cause a linear increase in *C* and a non-linear increase in *k* (Hillel, 2004). If increasing moisture content would cause an increase in *k* with a higher rate in comparison with *C*, then, α would increase with increasing moisture content. But, if increasing

a. moisture content: 0%

b. moisture content: 5%

c. moisture content: 10%

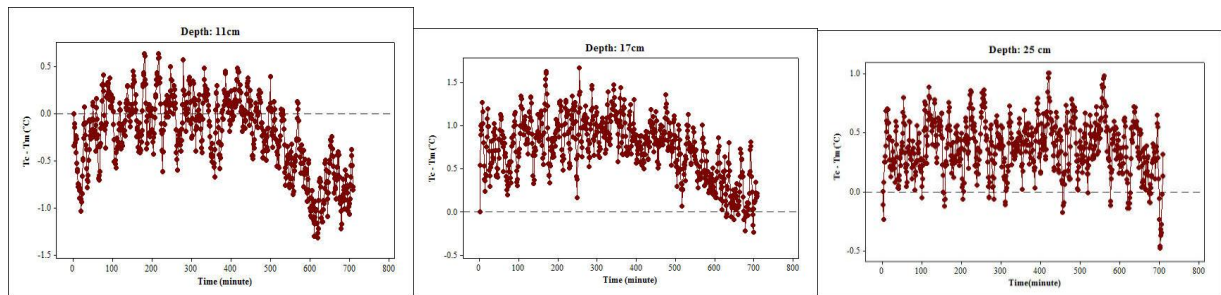d. moisture content: 15%

e. moisture content: 20%
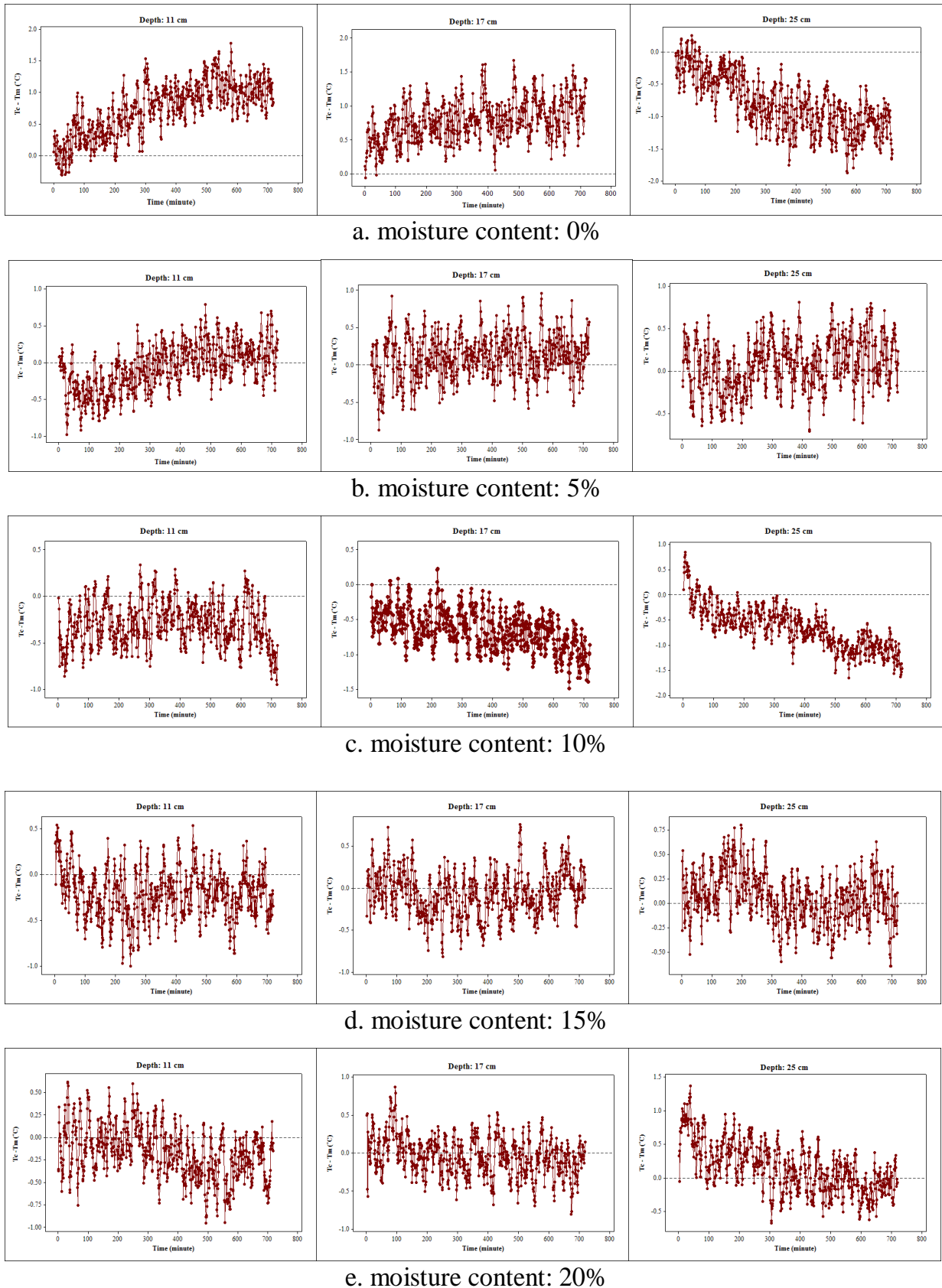
Figure 2. The differences between measured and predicted soil temperatures and time at 110, 170, and 250 mm depths for silty clay texture in different moisture contents.
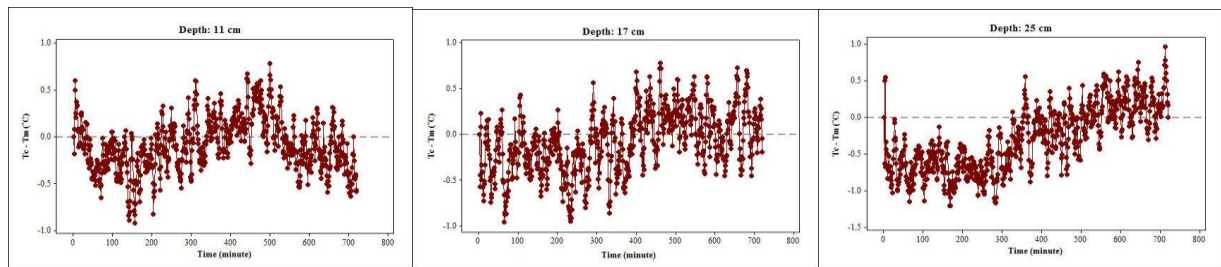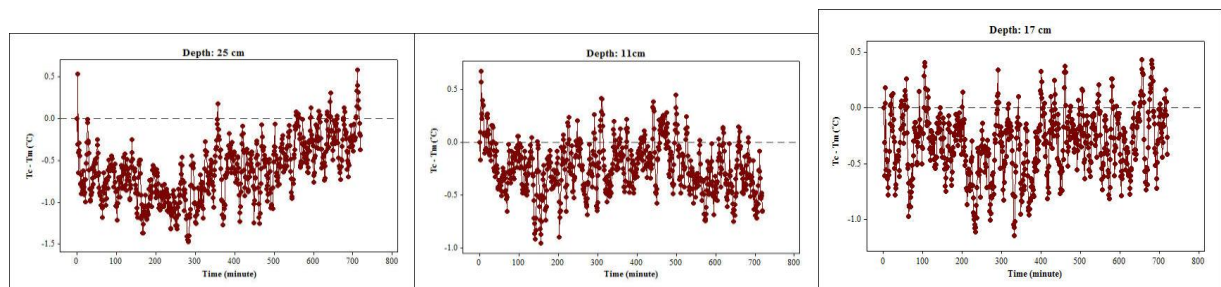
a. moisture content: 0%
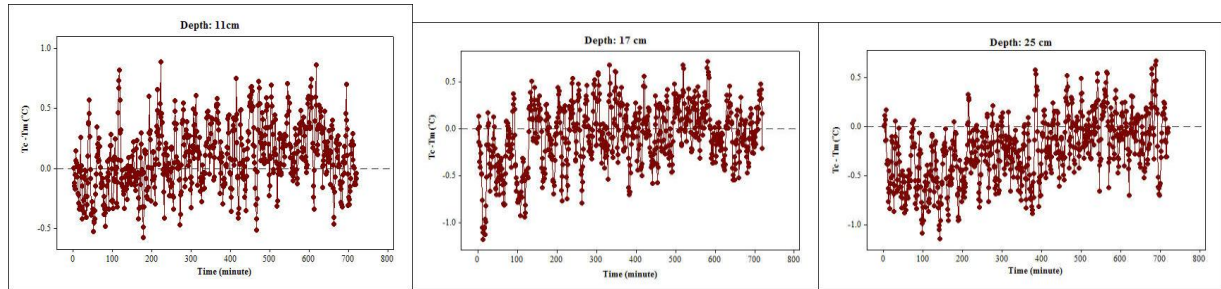
b. moisture content: 5%

c. moisture content: 10%

d. moisture content: 15%

e. moisture content: 20%

Figure 3. The differences between measured and predicted soil temperatures and time at 110, 170, and 250 mm depths for sandy texture in different moisture contents.

moisture content would increase C at a higher rate than k, then, it would cause α to decrease. The reason for the difference between the 2 textures soils in the moisture content was that the highest value of α occurred when water acted as a bridging agent among the soil grains. By gradual increase in soil moisture content, for achieving the maximum value of α, less mass of water was needed in sandy soil than silty clay as shown in Figures 1a and b; the specific surface area in silty clay soil was higher than the sandy soil.

Therefore, the sandy soil had less porosity compared to silty clay and thus, needed less water filling of the voids to improve its heat conductivity. RMSE values showed the magnitude of errors in determining α and MBE and also showed the tendency of the errors in overestimating or underestimating the results by the model. The sources of error producing RMSE are partly due to the error of temperature measuring sensors and the unsatisfying conditions needed for solution of the heat conductivity equation in experimental model. This may include non-uniformity or non-homogeneity in soil compaction, moisture content, and/or evaporation from the top soil surface. A minor part of the errors may be due to round off error and truncation error in the numerical solution.

Regarding the soil temperature predictions, as mentioned before, the range of the difference between predicted and measured values in most cases was between -1 and +1°C. This range of error can be considered as acceptable because the maximum intrinsic error of the thermal sensors was ±0.7°C. Also, there was absence of a clear trend increase in the errors with time in the 12 h time period in most of the cases. It can be concluded that the difference between predicted and measured values in time period of 12 h was due to the random and experimental errors and then the performance of the model to soil temperature prediction in the time period and can be considered as an acceptable error.

Conclusion

The main objectives of the present research were the application of numerical method in determining the soil thermal diffusivity with different textures and moisture contents and the evaluation of the adequacy of the method in soil temperature prediction. Results showed that the numerical method can be used for the determination of soil thermal diffusivity with an appropriate degree of accuracy and low RMSE values. Soil thermal diffusivity varied with respect to moisture content, in a way that up to a certain point it increased and then decreased. This point corresponded to higher moisture content for finer grained soils. In the prediction of soil temperature, with respect to the high frequency of differences between calculated and measured values in range of ± 1°C for a time period of 12 h, the acceptable

performance of the numerical method in prediction of soil temperatures was concluded.

ACKNOWLEDGEMENTS

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