Estimating Soil Thermal Properties from Sequences of Land Surface Temperature Using Hybrid Genetic Algorithm-Finite Difference Method

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Abstract

Most models used in land surface hydrology, vadose zone hydrology, and hydro-climatology require an accurate representation of soil thermal properties (soil thermal conductivity and volumetric heat capacity). Various empirical relations have been suggested to estimate soil thermal properties. However, they require many input parameters such as soil texture, mineralogical composition, porosity and water content, which are not always available from laboratory experiments and field measurements. In this paper, to overcome the above challenge, a hybrid numerical method, Genetic Algorithm-Finite Difference (GA-FD), is proposed to estimate soil thermal properties using land surface temperature (LST) as the only input. The genetic algorithm (GA) optimization method coupled with the finite difference (FD) modeling technique is a viable hybrid approach for estimating soil thermal properties. The finite difference method is employed to solve the heat diffusion equation and simulate LST, while a robust optimization technique (GA) is used to retrieve soil thermal properties by minimizing the difference between observed and simulated LST. Furthermore, a generalization of the hybrid model is developed for inhomogeneous soil, in which soil thermal properties are not constant throughout the soil slab. The proposed model is applied to the First International Satellite Land Surface Climatology Project (ISLSCP) Field Experiment (FIFE). The results show that the proposed hybrid numerical method is able to estimate soil thermal properties accurately, and therefore effectively eliminate the need for the unavailable soil parameters which are required by empirical methods for determining the soil thermal conductivity and volumetric heat capacity. Remarkably, the temporal variation of the retrieved soil thermal conductivity is consistent with the volumetric water content, even though no water content information is used in the model.

Keywords: Genetic Algorithm-Finite Difference model; soil thermal properties; Land surface temperature.

1. Introduction

Knowledge of the soil thermal properties (thermal conductivity and volumetric heat capacity) is required for the accurate prediction of soil temperature and its influence on surface-energy partitioning (Peters-Lidard et al., 1998; Alkhaler et al., 2011), soil nitrification or de-nitrification, the production and release of greenhouse gases from soil (Van Bochove et al., 2001; Nkongolo et al., 2010), plant and crop growth rates (Nagai and Makino, 2011), soil water retention and unsaturated hydraulic conductivity (Hopmans and Dane, 1986; Andry et al., 2009), timing and rate of snowmelt (Lynch et al., 1998; Niu et al., 2006), chemical processes in soil (Hopmans et al. 2002), and soil water vapor flow in coupled water and heat transport (Nassar and Horton, 1992; Bittelli et al., 2008).

In situ measurement of soil thermal conductivity (λ) and volumetric heat capacity (c) can be conducted by various methods, namely the Needle Probe (Herzen and Maxwell, 1959; Lister, 1979; Brigaud and Vasseur, 1989; Waite et al., 2002; Riche and Schneebeli, 2010), Divided Bar (Birch, 1950; Sass et al., 1984; Mottaghy, 2008), Borehole relaxation (Wilhelm, 1990; Verma, and Andaverde, 2007), heat pulse probe (Silliman and Neuzil, 1990; Bristow, 1998), and thermal gradients (Somerton, 1992). These available measurement techniques are mainly time-consuming, costly, and labour-extensive. As a result, earlier hydrologic campaigns have not measured them as rigorously as the other hydro-climatic driving factors such as precipitation, topography, and vegetation despite their importance. Because of the lack of measured soil thermal properties, researchers regularly approximate them in different ways and then associate any errors or uncertainties in model predictions with their soil thermal estimates (Mohanty et al., 2002).

Because of difficult and time-consuming *in situ* measurement procedures and also relatively high cost of measuring instruments, a number of studies have tried to develop empirical relations to estimate soil thermal conductivity based on the influential factors such as soil texture, water content, temperature, and porosity (De Vries, 1963; Farouki, 1986; Chung and Horton, 1987; Hopmans et al., 2002; Usowicz et al., 2006, 2008; Murray and Verhoef, 2007; Lu et al., 2007, 2009; Tranawski et al., 2009). Similarly, soil volumetric heat capacity has been estimated from knowledge of soil porosity and the soil organic, mineral, and water content through empirical equations (De Vries, 1963; Campbell, 1985; Ren et al., 2003; Lu et al., 2009). These empirical expressions require very specific and/or exhaustive input parameters which are not always routinely available (this was certainly the case in the present study). Moreover, most of these empirical models are valid only for a specific range of soil

moisture and temperature and a particular soil type, and thus cannot be used widely. Erzin et al. (2008) stated that the existing empirical relations are not accurate enough and developed an artificial neural network model to predict soil thermal properties for clayey, silty, and sandy soils. They used soil water content, dry density, and grain size distribution as inputs to their proposed neural network model. In another attempt, Nicolsky et al. (2009) developed a variational data assimilation model to estimate soil thermal properties from the soil temperature records, but their model works well only for fully saturated soils.

To overcome the aforementioned deficiencies associated with the empirical and variational data assimilation models of estimating soil thermal properties, we have introduced a new methodology to estimate soil thermal properties from easily measurable land surface temperature (LST). The approach developed in the context of this research used an optimization method (genetic algorithm) coupled with a finite difference modeling technique to estimate soil thermal properties. Unlike the available empirical and/or neural network-based approaches, the new model does not need the inaccessible input data such as soil water content, porosity, and grain size distribution. It can also be applied over a wide range of soil moistures.

Sequences of land surface temperature (LST) measurements are used as the only input and estimate soil thermal properties by minimizing an objective function describing the difference between measured and simulated LST. Therefore, the main superiority of the proposed model over the available methods of estimating soil thermal properties is the fact that it requires only LST measurements. The objective (fitness) function can be minimized by using a suitable nonlinear optimization technique (e.g., the steepest descent method, Gauss-Newton method, conjugate gradient method, etc.). However, these traditional non-linear optimization techniques are inefficient, or prone to converging to local optima, and often pose a convergence problem. Consequently, in the recent past, the traditional non-linear optimization techniques have been criticized by several researchers (Gentry et al., 2001; Ng and Perera, 2003; Jha et al., 2004; Keedwell and Khu, 2005; Cengiz and Tokat, 2008; Niknam et al., 2010) and non-conventional optimization techniques such as genetic algorithm (GA) and genetic programming have attracted the attention of various researchers including the hydrologists (Wang, 1991; Simpson et al., 1994; Savic et al., 1999; Reed et al., 2000; Ng and Perera, 2003; Wang and Zheng, 2007; Sen and Oztopal, 2010).

A particular advantage of GA is its insensitivity to the initial guess values of the parameters (i.e., variables) to be optimized. Unlike the traditional optimization techniques, GA searches from a population of points, and not from a single point, and thus is less prone to get ‘stuck’ at local optima

than gradient search or other traditional optimization methods. Hence, a properly designed GA ensures global optimal or at least near-optimal solutions to optimization problems. Therefore, in this study, GA is used to minimize the objective function. Since the objective function minimizes the difference between observed and simulated LST, the relevant system equation is the heat diffusion equation. A very robust approach for solving the heat diffusion equation includes the use of numerical methods. One class of numerical methods that is extremely popular involves finite difference (FD). Herein, the FD technique which can effectively model the inhomogeneity within the soil is utilized to solve the heat diffusion equation and simulate LST.

The literature describing the applications of the hybrid GA-FD method to engineering problems is not abundant. To the authors' best knowledge, there are only a number of applications of GA-FD to engineering problems. Karr et al. (2000) solved inverse initial-value, boundary value problems through combination of GA and FD. Gentry et al. (2003) employed a hybrid GA-FD approach for locating highly probable areas of leakage based upon aquifer head data near the suspected leakage area. Chen et al. (2005) formulated microwave imaging of buried objects as an inverse problem and used the coupled GA-FD method to determine the location and dimensions of two-dimensional inhomogeneous objects buried in soil. Kim and Baek (2007) proposed a combined GA-FD technique to analyze the inverse radiation problem in a cylindrical geometry. In their inverse radiation problem, boundary conditions such as temperature distribution and emissivity were estimated given the measured incident radiative heat fluxes. Ding et al. (2007) developed a mixed GA-FD model for optimal design of ultra wideband antennas. Infantolino et al. (2009) used a GA algorithm in conjunction with a FD method to determine an optimal position of an antenna on a platform. Awad et al. (2011) used a combined GA-FD method for the optimal removal of heavy metals pollutant from groundwater.

In this paper the efficiency of the hybrid GA-FD method is examined for estimating the soil thermal properties from the LST time series. The FD approach is employed to calculate LST, then GA is used to estimate soil thermal properties by minimizing an objective function representing the difference between observed and calculated LST. The applicability, adequacy and robustness of the developed model are tested using the area-averaged Betts and Ball (1998) dataset from the First International Satellite Land Surface Climatology Project (ISLSCP) Field Experiments (FIFE) across a prairie region in Kansas.

2. Methodology

2.1. Heat Diffusion Equation

Assuming that soil is homogeneous and heat flow is in the vertical direction only, the governing equation that describes the vertical diffusion of heat into an underlying soil is the heat diffusion equation, shown as follows:

$$c \frac{\partial T(z,t)}{\partial t} = \lambda \frac{\partial^2 T(z,t)}{\partial z^2} \quad (1a)$$

$$T(z, t_0) = f_1(z) \quad (1b)$$

with boundary conditions

$$\lambda \left. \frac{\partial T(z,t)}{\partial z} \right|_{z=0} = -G(t) \quad (2a)$$

$$T(z = 0.5m, t) = \bar{T} \quad (2b)$$

where $T(z,t)$ is the soil temperature at depth z and time t , $G(t)$ is the ground heat flux or surface boundary forcing and $\bar{T}$ is the deep soil temperature (herein deep soil is taken at $z = 0.5$ m). The initial condition, $f_1(z)$, includes soil temperature values for each node in the soil column at the beginning of the simulation (time t_0).

In this study, measurements of soil temperature at $z = 0.5$ m, and ground heat flux are used for the lower and upper boundary conditions, respectively. Even for cases, in which the ground heat flux (G) and deep soil temperature ($\bar{T}$) haven't been measured, LST observations can be used to retrieve them. The diurnal amplitude of the soil temperature is the maximum at the surface and decreases exponentially with depth. At a depth of 0.3-0.5 m, diurnal soil temperature amplitude is negligible and at these depths soil temperature can be considered constant over a day (Hu and Islam, 1995; Hirota et al., 2002). Caparrini et al. (2003) presented a simple approach for the estimation of the daily constant deep soil temperature using a semi-diurnal filter of LST measurements. Furthermore, Wang and Bras (1999) developed a method that allows the ground heat flux, G , to be computed from the corresponding time series measurement of LST. If the ground heat flux (upper boundary condition) and deep soil temperature (lower boundary condition) are not available from *in situ* measurements, the

Wang and Bras (1999), and Caparrini et al. (2003) studies can be used to estimate them from the LST observations. Thus, we could say that the LST measurement is the only input to the model.

2.2. Numerical Model (Finite Difference)

To obtain meaningful results from a numerical approximation, a model must be well posed. The prerequisites of a well-posed model are that it conforms to the three basic requirements of (1) existence; (2) uniqueness; and (3) stability (Bear, 1972; Gentry et al., 2003). Uniqueness plays a particularly important role for the technique presented in this paper.

The heat diffusion equation is solved using an implicit finite difference scheme. This leads to a vector propagation equation that calculates the temperature for a set of discrete depths and time steps starting from a discretized initial condition. The resulting equations for the interior nodes of the numerical model, with a time interval of Δt , and a uniform grid with a spacing of Δz , is shown in Eq. (3). When implementing the finite difference scheme, boundary conditions must be treated in a special manner. A modified form of the approximation equation is used for nodes adjacent to the defined top (Neumann) and bottom (Dirichlet) boundaries, see Eqs. (4a), and (4b).

$$-\alpha T_{i-1}^{n+1} + (1 + 2\alpha)T_i^{n+1} - \alpha T_{i+1}^{n+1} = T_i^n, \quad i = 2, \dots, N-2 \quad (3)$$

$$(1 + \alpha)T_i^{n+1} - \alpha T_{i+1}^{n+1} = T_i^n + \frac{\Delta t}{c\Delta z} G^{n+1}, \quad i = 1 \quad (4a)$$

$$-\alpha T_{i-1}^{n+1} + (1 + 2\alpha)T_i^{n+1} = T_i^n + \alpha \bar{T}^{n+1}, \quad i = N-1 \quad (4b)$$

where $\alpha = \frac{\lambda}{c} \frac{\Delta t}{\Delta z^2}$, i is the node number, n is the time step, T_i^n is the numerical value of the soil temperature at depth $i\Delta z$ and at time $n\Delta t$, and N is the number of layers within the grid.

In this study, a 0.5 m soil column is discretized into $N = 50$ layers with the thickness of $\Delta z = 0.01$ m. Given the half-hourly temporal resolution of ground heat flux and soil temperature measurements, the model was run with a half-hourly time step (i.e., $\Delta t = 30$ min). The FD method is employed to compute land surface temperature because it can effectively and easily model the inhomogeneity within the soil and hence allows generalizing the model for an inhomogeneous soil slab.

2.3. Genetic Algorithm

Genetic algorithm (GA) is a heuristic global searching technique introduced by Holland (1975) and since then it has been successfully applied to numerous complex search problems (Goldberg, 1989). It mimics the mechanism of natural selection according to the survival and adaptation biological processes to find near-optimal solutions in a search space. Traditionally, the GA starts with the initial population of binary bits (i.e., 0's and 1's) strings generated in a random way. These binary strings of specific length can encode integers, real numbers, or any potential solutions to the problem, and are taken from the problem search space that includes all the available solutions. The performance of these strings is evaluated by decoding them into a search space and computing the fitness value for each of them with respect to an objective function. Fitness value is an indicator of the quality of each string in the problem's domain. After all strings are evaluated, a new, better population will be created through a set of genetic operators.

The most common genetic operators are: (1) reproduction (selection), (2) crossover (mating), and (3) mutation. In the reproduction process, individual strings are copied from one generation into the next based on their relative fitness value with respect to the population's fitness value. The fitness value is calculated by an evaluation function that indicates how well each string performs in the problem's domain. The fitness of each string represents its survival potential and reproductive capability in the next generations. Therefore, reproduction strings with low fitness values are eliminated from the population, while high-fitness strings have better chance of contribution in the subsequent generation. There are different techniques to relate a string's fitness to its probability of selection, namely fitness proportionate selection, remainder stochastic sampling with and without replacement, stochastic sampling with and without replacement, deterministic sampling, and stochastic tournament (Goldberg, 1989). In this study, the fitness proportionate selection technique is chosen for reproduction because of its popularity. This technique picks a string with a probability proportional to its fitness value. Thus, a higher probability of selection (P_i) is given to a string with greater fitness value according to the following relation:

$$P_i = \frac{f_i}{\sum_{i=1}^m f_i} \quad (5)$$

where f_i is the fitness of string i , and m is the population size.

It is clear from the above discussion that the high-quality solutions will acquire high probabilities, while the low-quality solutions will obtain small probabilities of existence in the next generation.

Therefore, reproduction takes out the weak strings from the next generation, but increases the presence of fittest members to the next generation.

After reproduction, newly reproduced strings in the mating pool are mated through a crossover process. Crossover follows reproduction and is a means that allows the two high-fitness strings (parent) to produce two offspring by swapping portions of their structures based on a random process with specific probability. Crossover proceeds in two steps: First, two newly reproduced strings are chosen randomly for mating from the mating pool. Then, a crossover site is selected for these two strings at random, and the bits of the two strings are exchanged from the crossover site. This is referred to as single-point crossover scheme. The two resulting strings have the characteristics of their parents, are called “children” and are members of a new population. Crossover between the two parent strings takes place with a certain probability, referred to as crossover probability (p_c). A crossover probability of p_c implies that only $100 \times p_c$ percent of strings in the population take part in the crossover process and the remaining $100 \times (1 - p_c)$ percent of the population will be untouched. The crossover probability is normally set a value so that the crossover is implemented on most of the strings in the population. The parent strings which do not experience mating, will be copied into the next generation unaltered. The final result of the crossover genetic operator is the creation of a new population as large as the old population which includes mainly offspring (children) strings, and a minority of parent strings that did not mate and remained unchanged. Reproduction and crossover provide the GA much of its searching capability. The GA selects good points in the previously specified search space via reproduction, and takes advantage of them to generate new points through crossover in order to hopefully create a population containing the fittest individuals.

Finally, mutation operation is applied occasionally, and randomly changes the value of a bit. Mutation changes the value of ‘0’ to a ‘1’ and vice versa, and thus is an important process that introduces new members to the population. In fact, mutation is a genetic operator applied with a small probability, and increases the population’s diversity in order to ensure that no point in the search space has a zero probability of being evaluated (Mousavi et al., 2007). This is particularly important since mutation enables the GA to converge to the optimum solution, even if the initial population is far from the optimal solution. Having said that, it is evident that choosing an appropriate value for the mutation probability (p_m) has a vital role on the performance of the GA (Koumouis and Georgiou, 1994; Samuel and Jha, 2003). DeJong (1975) showed that a mutation probability inversely proportional to the population size is adequate to prevent the GA to get stuck at local optima. The population takes its

ultimate form in the current generation after crossover and mutation. Thereafter, by decoding the strings in the current generation their fitness values will be calculated. The new population is used to create other populations through subsequent generations. After a number of generations, these genetic processes (i.e., reproduction, crossover, and mutation) will yield a population with very satisfactory solutions to the physical problem (i.e., highly fit strings in the domain).

Based on the above discussions, the population size, the probability of crossover, and the probability of mutation are the basic parameters that control the performance and convergence of the GA. Therefore, suitable values for these parameters should be chosen in order to ensure the robust performance of the algorithm. The literature shows that for a large number of problems a population size of 50 or more, a probability of crossover 0.6 to 0.9, and a probability of mutation 0.01 or less are good estimates for an initial run (Goldberg, 1989; Koumoussis and Georgiou, 1994). In this study, we observed that very good results could be obtained from the common GA parameters (Table 1).

[Table 1 near here]

The technique presented in this paper combines GA with the finite difference numerical scheme. The search variables in the context of this research are the soil thermal properties. The thermal properties are mapped from the FD numerical model to GA by encoding the variable into a string format and from GA to FD by decoding the string into its corresponding numerical representation. Furthermore, a flowchart of the specific GA-FD components used in this paper is provided in Fig 1. This technique is applied to the FIFE field data, where the measurement of LST time series exists.

[Figure 1 near here]

2.4. Fitness Function

Gentry et al. (2001) evaluated several varieties of objective functions to examine the performance of GA technique. It was discovered that the various forms of the fitness functions could force premature convergence of the solutions to a suboptimal area of the search space. A conventional L_2 norm or generalized L_2 norm is commonly used for the inverse problems (Sun, 1994; Gentry et al., 2001, 2003; Zeng et al., 2011). In this study, the conventional form of L_2 norm was used to represent the

fitness function. The design of the fitness function was based upon a realistic evaluation of the type of data that would be available in the typical field studies. The most likely data available to an investigator would be land surface temperature. The fitness function in this research was the square root of the sum of squared differences between observed and predicted LST (L_2 norm), as shown in the following equation:

$$F = \text{Min} \sqrt{\sum_{t=1}^M (T_o[t] - T_c[t])^2} \quad (6)$$

where $T_o[t]$ is the observed land surface temperature at time t , $T_c[t]$ is the computed LST at the same time using a suitable approach (Finite Difference), M is the total number of LST observations, and F is the fitness function. The target was to minimize the fitness function (Eq. 6). Suitable termination criteria must be specified in order to stop the hybrid numerical method. The GA-FD computer program developed in this study stops when the criterion $F = 1$ °K is satisfied or if the iteration (number of generations) reaches a specific value (Table 1).

3. FIFE Data

The model is tested over the FIFE field experiment where the measurements of ground heat flux and LST data are available. The longest contiguous days of the FIFE experiment (from Julian days 148 to 242 in 1987 and 160 to 243 in 1988) are used for the model validation. Measurements of ground heat flux and soil temperature at surface and different depths were reported every 30 min (48 observations per day). The Betts and Ball (1998) dataset used here is area-averaged based on several stations over the 15 km by 15 km study area. During the summers of 1987 and 1988 the number of deployed instruments and measurement stations (including their locations) changed considerably. The Betts and Ball (1998) dataset applies quality-control and weighted-averaging procedures to produce the area-effective data.

To evaluate the performance of the GA-FD model an error analysis was made based on mean-absolute error (MAE), root-mean-square error (RMSE), and determination coefficient (R^2) of the linear regression line between the predicted values from the model and the observed soil temperature. The equations for MAE, RMSE and R^2 are:

$$\text{MAE} = \frac{1}{M} \sum_{t=1}^M |T_o[t] - T_c[t]| \quad (7)$$

$$\text{RMSE} = \sqrt{\frac{\sum_{t=1}^M (T_o[t] - T_c[t])^2}{M}} \quad (8)$$

$$R^2 = 1 - \frac{\sum_{t=1}^M (T_o[t] - T_c[t])^2}{\sum_{t=1}^M (T_o[t] - \bar{T}_o)^2} \quad (9)$$

where $\bar{T}_o$ is the average of observed soil temperatures. Lesser values of MAE and RMSE indicate better agreement between the estimated and measured values.

Castelli et al. (1999) reported values of $0.46 \text{ (J m}^{-1} \text{ K}^{-1} \text{ s}^{-1})$ and $2.3 \times 10^6 \text{ (J K}^{-1} \text{ m}^{-3})$ respectively for the soil thermal conductivity and volumetric heat capacity of FIFE field experiment. The soil heat diffusion equation was solved using the reported soil thermal properties values. Figures 2 and 3 show the comparison between measured and predicted soil temperature at the land surface and $z = 0.05 \text{ m}$ for FIFE 87 and 88, respectively. As illustrated, there is a considerable difference between the measured and estimated soil temperature in both years. This difference occurs because of the erroneous reported soil thermal properties values, and therefore it is necessary to estimate the correct values of these parameters. For FIFE 87, the model overpredicts the soil temperature while for FIFE 88 the estimated soil temperatures are closer to the measurements, but the amplitude of estimated soil temperatures is less than that of observations. It is evident in these two figures that the soil thermal properties have a significant effect on the magnitude and amplitude of predicted soil temperature.

[Figure 2 near here]

[Figure 3 near here]

4. Model Tests at FIFE

The GA-FD initiates the search with a randomly generated set of solutions that may or may not be feasible. As the GA-FD run progresses, the infeasible solutions are eliminated because the penalties assigned to them reduce their fitness, making their chances slim for selection in the next generation. At

the end of a run, a large number of feasible and near-optimal solutions are obtained. Fig. 4 shows the RMSE of LST prediction versus generation number (iteration). λ and c are adjusted in each generation number to minimize the error in the LST estimation. The continuous decrease toward an asymptotic minimum of land surface temperature RMSE is evident. By the end of about 20 generations, LST RMSE reduces only slightly. At this point, the common assumptions of the model (e.g., temporally constant soil thermal properties, constant soil thermal properties throughout the soil column, etc.) as well as observations errors do not allow the iteration scheme to further decrease the misfit between estimated and observed LST. The GA-FD was run for 50 generations, although the improvement has been found to be very small after about 20 generations.

[Figure 4 near here]

To estimate soil thermal properties, various tests have been done by the GA-FD model. In the first test, it is assumed that the soil thermal conductivity and volumetric heat capacity are spatially (throughout the soil medium) and temporally (for each year during the FIFE experiment) constant. The predicted λ and c values were respectively $1.58 \text{ (Jm}^{-1}\text{K}^{-1}\text{s}^{-1}\text{)}$ and $0.92 \times 10^6 \text{ (JK}^{-1}\text{m}^{-3}\text{)}$ for FIFE 87 and $0.65 \text{ (Jm}^{-1}\text{K}^{-1}\text{s}^{-1}\text{)}$ and $0.82 \times 10^6 \text{ (JK}^{-1}\text{m}^{-3}\text{)}$ for FIFE 88 (Table 2). Unfortunately, measurements of the soil thermal properties are not available in Betts and Ball (1998) dataset. To test the performance of the developed hybrid model, the soil heat diffusion equation was solved using the retrieved soil thermal properties from the GA-FD model. Then, the predicted soil temperatures at surface ($z = 0 \text{ m}$) and depth of 0.05 m ($z = 0.05 \text{ m}$) were compared with observations (Table 2). For the reported thermal properties by Castelli et al. (1999), the RMSE of FIFE 87 LST prediction is $8.14 \text{ }^\circ\text{K}$, compared to the RMSE of $2.93 \text{ }^\circ\text{K}$ using the optimum soil thermal properties retrieved by the GA-FD technique.

[Table 2 near here]

In the other three tests, the inhomogeneity through the soil slab (i.e., the vertical variation of thermal properties) is investigated. To consider the effect of inhomogeneity, the soil slab with the total thickness of 0.5 m was divided into two, five, and ten sub-layers of equal thickness in three different numerical experiments (Table 2). It is assumed that thermal properties are constant within each sub-layer, but they can be different from the thermal properties of other sub-layers. Similar to the assessment of the one-layer model performance, the soil heat diffusion equation was solved with the

predicted soil thermal properties from the two-layer, five-layer, and ten-layer models and the estimated soil temperatures were compared to measurements based on MAE, RMSE, and R^2 (Table 2). As indicated, by increasing the numbers of sub-layers within the soil slab the optimization results tend to slightly improve and the corresponding RMSE decreases. This implies that the model can assist in predicting changes of soil thermal properties through the soil. To have a better understanding of model performance, the plot of observed and estimated LST from the ten-layer GA-FD model is shown in Fig. 5 for FIFE 87 and 88. As shown, the model can retrieve soil thermal properties, and consequently soil temperature accurately.

[Figure 5 near here]

As a further test of the robustness of the model, the estimated soil temperature values at $z = 0.05$ m were compared with the corresponding measurements, which were withheld from the calculation for independent verification (Fig. 6). As illustrated, the soil temperature prediction is reasonably accurate, with the RMSE of 1.35 °K for FIFE 87 and 2.10 °K for FIFE 88 (for FIFE 88, the large scatter in a few soil temperature values results from errors in measurements). The measured and predicted values are consistent both in terms of values and day-to-day dynamics across the modeling period, indicating that the GA-FD model is able to predict soil thermal properties accurately. Accounting for the inhomogeneity within the soil slab reduces the RMSE of the soil temperature estimation at $z = 0.05$ m (Table 2).

[Figure 6 near here]

5. Temporal Variation of Soil Thermal Conductivity

Among the soil thermal properties, the thermal conductivity is most widely used in numerous meteorological and engineering applications. Consistent estimates of the thermal conductivity are useful in understanding the nature of soil thermal evolution and its influence on the microclimate and plant growth (Usowicz et al., 2006). Among the many factors such as soil water content, mineral composition, temperature, and porosity that influence thermal conductivity (λ), water content is the most variable one under field conditions and has the most significant role. Normally, dry soils exhibit low thermal conductivity because air, a poor conductor, separates the solid grains. If the moisture content of the soil increases, then the thermal conductivity rises because water is a good conductor. As

such, a moist soil has a higher thermal conductivity. To demonstrate that the GA-FD method is able to capture the functional dependence of soil thermal conductivity on water content, a numerical experiment was conducted. For this purpose, the one-layer GA-FD model was run for weekly intervals. In other words, we tried to estimate optimal soil thermal conductivity for each week rather than the whole period. The estimated values of thermal conductivity are shown in Fig. 7 as dashed lines. Weekly precipitation is also shown in the same figure as bars. As seen, the values of λ follow precipitation and dry down events in a consistent manner. Soil thermal conductivity (λ) increases with the accumulation of significant rain amounts, and it decays during an extended dry down event. As shown, the temporal variation of estimated thermal conductivity is consistent with the rainfall and dry down events, even though no information on soil water content and/or rainfall was used in the model.

[Figure 7 near here]

The weekly predicted soil thermal properties are used to solve the heat diffusion equation. Fig. 8 indicates the comparison between the estimated soil temperatures at $z = 0.05$ and the measurements. The plots show that the modeled and measured soil temperature at $z = 0.05$ m agree well, with the RMSE of 1.52 °K and 1.83 °K for FIFE 87 and 88, respectively. The statistical evaluations indicate the high accuracy of the GA-FD model in predicting soil thermal properties because soil temperature measurements at $z = 0.05$ m are not used in the optimization scheme, and thus provide a unique opportunity for independent verification of soil thermal properties retrievals. Comparing the RMSE of soil temperature prediction at $z = 0.05$ m with that of the time-invariant one-layer GA-FD model in Table 2 indicates that the predictions improve by taking into account the temporal variation of soil thermal properties.

Finally, the average of weekly λ values is computed and compared with that of the time-invariant one-layer GA-FD model in Table 2. The average of λ is 1.90 ($\text{J m}^{-1} \text{K}^{-1} \text{s}^{-1}$) for FIFE 87, and 0.77 ($\text{J m}^{-1} \text{K}^{-1} \text{s}^{-1}$) for FIFE 88. Corresponding λ values in Table 2 are 1.58 ($\text{J m}^{-1} \text{K}^{-1} \text{s}^{-1}$) and 0.65 ($\text{J m}^{-1} \text{K}^{-1} \text{s}^{-1}$) which are close to the average of weekly λ values. This closeness indicates that the GA-FD model is robust with respect to the estimation of λ .

[Figure 8 near here]

Conclusions

The accurate estimation of soil thermal properties is required in many agricultural and meteorological applications. It also has a significant impact on regulating surface energy fluxes and the prediction of soil temperature. Unlike previous studies, which rely mostly on empirical equations and need many input parameters, this study introduces a new technique for estimating soil thermal properties that overcomes the limitations of previous studies. The developed technique combines a numerical modeling technique (Finite Difference, FD) with an optimization method (Genetic Algorithm, GA) and uses LST as the only input. It also can be applied over a wide range of soil moisture and a soil temperature. The finite difference model is employed to solve the heat diffusion equation and estimate LST. Thereafter, the efficiency of a nontraditional optimization technique called genetic algorithm is assessed in predicting soil thermal properties by minimizing the difference between the observed and estimated LST from the finite difference model. The applicability, adequacy, and robustness of the developed model were tested using the FIFE dataset. The heat diffusion is solved using the retrieved soil thermal properties from the GA-FD model. It was observed that the estimated soil temperatures at the surface and $z = 0.05$ m are very close to the measurements. This proves that the GA-FD model is able to estimate soil thermal properties accurately, especially because soil temperature measurements at $z = 0.05$ m are withheld from the optimization scheme for independent validation of retrieved soil thermal properties.

In addition, the developed model was generalized to take into account inhomogeneity through the soil slab. The generalized model divides the soil slab into sub-layers and estimates soil thermal properties within each sub-layer individually (i.e., the soil thermal properties of each layer are estimated independently). The results improve as the model accounts for the soil inhomogeneity. Finally, we demonstrated that the GA-FD model is capable of showing the functional dependence of soil thermal conductivity on the volumetric water content even though no information on soil water content or rainfall was used as input.

Overall, the GA-FD model is robust, reliable and efficient in estimating soil thermal properties from the LST data. With the current availability of high speed and large memory PCs, the use of GA-FD scheme is recommended for determining soil thermal properties from the LST measurements instead of the empirical methods (e.g., Usowicz et al., 2008;; Lu et al., 2009) and/or neural network-based approaches (e.g., Erzin et al., 2008), which require exhaustive input parameters which are not always routinely available

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Figure Captions:

- Fig. 1. Flowchart of the proposed hybrid genetic algorithm-finite difference method.
- Fig. 2. Comparison between observed and estimated soil temperature at land surface and $z = 0.05$ m using soil thermal properties reported by Castelli et al. (1999) for FIFE 87. (top) Scatterplots of half-hourly soil temperature, (bottom) Time series for Julian days 148-177.
- Fig. 3. Comparison between observed and estimated soil temperature at land surface and $z = 0.05$ m using soil thermal properties reported by Castelli et al. (1999) for FIFE 88. (top) Scatterplots of half-hourly soil temperature, (bottom) Time series for Julian days 160-190.
- Fig. 4. Decrease of LST RMSE versus the generation number.
- Fig. 5. Comparison between observed and estimated LST using soil thermal properties retrieved by the ten-layer GA-FD model for FIFE 87 and 88. (top) Scatterplots of half-hourly soil temperature, (bottom) Time series for Julian days 148-177 of FIFE 87 and 160-190 of FIFE 88. ($z=0$)
- Fig. 6. Comparison between observed and estimated LST using soil thermal properties retrieved by the ten-layer GA-FD model for FIFE 87 and 88. (top) Scatterplots of half-hourly soil temperature, (bottom) Time series for Julian days 148-177 of FIFE 87 and 160-190 of FIFE 88. ($z = 0.05$ m).
- Fig. 7. Dashed line: Weekly predicted values of soil thermal conductivity. Histogram: Weekly precipitation. (top) FIFE 87, (bottom) FIFE 88.
- Fig. 8. Comparison of observed and estimated soil temperature at $z = 0.05$ m using weekly-varying soil thermal conductivity

Table Captions:

Table. 1. Typical GA parameters used in this study.

Table 2. Performance indices of GA-FD method for FIFE 87 and 88.

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Table. 1. Typical GA parameters used in this study.

Population size	100
Number of generation	50
Probability of crossover	0.7
Probability of mutation	0.01

Table 2. Performance indices of GA-FD method for FIFE 87 and 88.

Different Approaches		λ ($\text{Jm}^{-1}\text{K}^{-1}\text{s}^{-1}$)	c ($\text{JK}^{-1}\text{m}^{-3}$) $\times 10^6$	MAE (K)		RMSE (K)		R^2	
				Surface	$z = 0.05$ (m)	Surface	$z = 0.05$ (m)	Surface	$z = 0.05$ (m)
FIFE 87	Castelli et al. (1990)	0.46	2.30	7.30	6.27	8.14	7.11	0.77	0.67
	GA-FD (One layer)	1.58	0.92	2.42	1.47	2.93	1.84	0.83	0.84
	GA-FD (Two layers)	1.72 0.98	1.00 1.86	2.32	1.29	2.89	1.62	0.85	0.85
	GA-FD (Five layers)	1.62 2.17 0.89 2.75 1.97	0.86 2.73 2.31 1.93 2.47	2.22	1.12	2.77	1.42	0.88	0.89
	GA-FD (Ten layers)	1.52 3.22 3.04 0.49 2.99 2.62 3.15 3.39 1.74 1.58	0.80 0.87 3.08 2.58 0.95 2.36 1.70 1.52 3.01 1.74	2.10	1.05	2.61	1.35	0.89	0.90
	Castelli et al. (1990)	0.46	2.30	3.82	2.83	4.78	3.64	0.76	0.61
	GA-FD (One layer)	0.65	0.82	2.40	1.57	3.24	2.21	0.82	0.78
	GA-FD (Two layers)	0.65 0.44	0.80 0.95	2.40	1.53	3.24	2.18	0.83	0.78
	GA-FD (Five layers)	0.67 4.00 0.86 2.90 3.60	0.80 0.87 3.00 2.26 3.81	2.28	1.50	3.10	2.14	0.83	0.79
	GA-FD (Ten layers)	0.72 3.67 3.27 3.93 1.45 0.69 2.46 2.62 3.46 0.81	0.82 1.03 1.50 3.25 2.59 3.32 1.54 1.47 2.43 3.00	2.12	1.49	2.90	2.10	0.84	0.81