IN-SITU DETERMINATION OF SOIL THERMAL CHARACTERISTICS

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ABSTRACT

Four variations of the least-squares regression procedure proposed by Lettau (1971) were used to define a solution envelope containing the soil thermal diffusivity function, $\alpha(z)$, for a soil with a heterogeneous moisture profile. An explicit finite difference model of the one-dimensional heat equation was used to evaluate the four variations of Lettau's procedure based upon agreement between measured and simulated temperatures over a 24-h temperature cycle. The application of Lettau's regression procedure to a database containing only temperature data from the cooling cycle portion of the diurnal temperature wave was shown to most faithfully reproduce field temperature measurements. KEYWORDS. Soil, Temperature.

INTRODUCTION

Efforts to partition thermal energy transfer between the soil surface and the air into its sensible and latent components depend upon independent determination of the soil heat flux, an important component of the surface energy balance. Soil heat flux may be measured *in situ* using flat-plate heat flux transducers (Philip, 1961), or it may be estimated by combining laboratory determinations of the soil thermal conductivity, λ, with field measurements of the soil temperature gradient, $\delta T/\delta z$. Empirical methods of estimating the soil heat flux have been proposed by Oliver et al. (1987); Horton and Wierenga (1983); Novak and Black (1983); and Choudhury et al. (1987).

The use of the heat flux transducer can be impractical, especially in instances in which the soil thermal characteristics, soil moisture regimes, and incident solar radiation regimes vary spatially. Heat flux transducers are difficult to install and calibrate properly, and tend to interfere with the migration of soil moisture; when the conductivity of the flux plate material differs significantly from the conductivity of the soil in which it is installed, the transducer also disrupts the soil heat flux. A method to determine soil thermal conductivity *in situ* using simpler instrumentation would facilitate the measurement of soil heat flux.

The classical approach to the analysis of soil heat flux (Carslaw and Jaeger, 1959; Jackson and Kirkham, 1958; and Van Wijk, 1963) combines Fourier's Law:

$$q = -\lambda \frac{\delta T}{\delta z} \qquad (1)$$

with the Principle of Conservation of Energy,

$$q_i A_i - q_o A_o = \frac{\delta S}{\delta t} \qquad (2)$$

where

q	=	heat flux in the z-direction (W/cm²)
λ	=	soil thermal conductivity (W/cm C)
$\delta T/\delta z$	=	temperature gradient in the z-direction (C/cm)
q_i	=	heat flux entering a control volume of soil (W/cm²)
q_o	=	heat flux leaving a control volume of soil (W/cm²)
A_i	=	surface area through which incoming heat flows (cm²)
A_o	=	surface area through which outgoing heat flows (cm²)
$\delta S/\delta t$	=	time rate of change of heat storage in a control volume of soil (W)
Cp	=	soil volumetric heat capacity (J/cm³ C)

If heat flux is assumed to occur in only one direction, z, then a combination of Fourier's Law and the Principle of Conservation of Energy yields the one-dimensional heat equation, a parabolic partial differential equation of the form:

$$C_p \frac{\delta T}{\delta t} = \frac{\delta}{\delta z}\left(\lambda \frac{\delta T}{\delta z}\right) \qquad (3)$$

When the partial derivative on the right-hand side of equation 3 is expanded, the resulting form of the heat equation is:

$$C_p \frac{\delta T}{\delta t} = \lambda \frac{\delta^2 T}{\delta z^2} + \frac{\delta \lambda}{\delta z}\frac{\delta T}{\delta z} \qquad (4)$$

Equation 4 may then be rearranged to yield:

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$$\frac{\delta T}{\delta t} = \alpha \frac{\delta^2 T}{\delta z^2} + \beta \frac{\delta T}{\delta z} \qquad (5)$$

in which α is defined as the soil thermal diffusivity in cm²/s:

$$\alpha = \frac{\lambda}{C_p} \qquad (6)$$

and β is defined as:

$$\beta = \frac{1}{C_p} \frac{\delta \lambda}{\delta z} \qquad (7)$$

Equation 5 is the form of the heat equation used as Lettau's regression model. The two spatial derivatives of temperature, $\delta T/\delta z$ and $\delta^2 T/\delta z^2$, were treated as the independent variables, $\delta T/\delta t$ as the dependent variable, and α and β as the regression parameters.

The objective of this study was to evaluate the utility of four variations of the least-squares regression procedure proposed by Lettau (1971) for estimating the soil thermal conductivity as a function of depth, using the following tools:

- A model of the relationship between the soil volumetric heat capacity, C_p, and soil moisture content, θ.
- An explicit finite difference model of the one-dimensional expanded heat equation.

MODEL DEVELOPMENT
ESTIMATING THE SOIL VOLUMETRIC HEAT CAPACITY, C_p

The soil volumetric heat capacity was determined using a technique proposed by deVries (1963) and simplified by Campbell (1985):

$$C_p(\theta, \phi_f) = C_m(1 - \phi_f) + C_w \theta \qquad (8)$$

where
C_m = volumetric heat capacity of the mineral component of the soil (assumed to be 2.39 J/cm³ C)
C_w = volumetric heat capacity of water (assumed to be 4.18 J/cm³ C)
ϕ_f = soil porosity

The volumetric heat capacities of the mineral and organic fractions are very similar, typically 2.39 and 2.50 J/cm³ C, respectively, so the two fractions have been combined in the term $(1 - \phi_f)$. The soil porosity was calculated from soil bulk density measurements using the equation:

$$\phi_f = 1.00 - \left(\frac{BD}{PD}\right) \qquad (9)$$

where BD is the soil bulk density (g/cm³), and PD is the soil particle density, assumed to be 2.65 g/cm³, a typical value for quartz and clay minerals (Campbell, 1985).

APPROXIMATION OF PARTIAL DERIVATIVES

The first task in developing the finite difference model of equation 5 was the algebraic approximation of the partial derivatives. The first partial of temperature with respect to time was expressed as follows (superscripts denote time step, subscripts denote space indices):

$$\frac{\delta T}{\delta t^i} = \frac{T_i^{j+1} - T_i^j}{\Delta t} \qquad (10)$$

The first and second partials of temperature with respect to space were defined by the explicit approximations:

$$\frac{\delta T}{\delta t}_i = \frac{2\left(T_{i+1}^j - T_{i-1}^j\right)}{2\Delta z_i + \left(\Delta z_{i+1} + \Delta z_{i-1}\right)} \qquad (11)$$

$$\frac{\delta^2 T}{\delta z^2}_i = \frac{2}{\Delta z_i}\left[\frac{\left(T_{i+1}^j - T_i^j\right)}{\Delta z_i + \Delta z_{i+1}} - \frac{\left(T_i^j - T_{i-1}^j\right)}{\Delta z_{i-1} + \Delta z_i}\right] \qquad (12)$$

The explicit finite difference equation that results from the above approximations is:

$$T_i^{j+1} = T_i^j + \frac{2\alpha\Delta t}{\Delta z_i}\left[\frac{\left(T_{i+1}^j - T_i^j\right)}{\Delta z_i + \Delta z_{i+1}} - \frac{\left(T_i^j - T_{i-1}^j\right)}{\Delta z_{i-1} + \Delta z_i}\right]$$

$$+ 2\beta\Delta t\left[\frac{\left(T_{i+1}^j - T_{i-1}^j\right)}{2\Delta z_i + \Delta z_{i+1} + \Delta z_{i-1}}\right] \qquad (13)$$

ESTIMATING THE PARTIAL DERIVATIVES FROM FIELD TEMPERATURE MEASUREMENTS

Using the expanded form of the heat equation as the regression model required the estimation of $\delta T/\delta t$, $\delta T/\delta z$, and $\delta^2 T/\delta z^2$ from field temperature measurements. To determine the two spatial derivatives, the depth-temperature profile at each time interval was fit with a cubic spline interpolating function composed of $(n - 1)$ cubics of the form:

$$T_i(z) = a_i z^3 + b_i z^2 + c_i z + d_i \qquad (14)$$

The end conditions selected for the spline model specified $\delta T/\delta z = 0$ and $\delta^2 T/\delta z^2 = 0$ at 95 cm. The first and second derivatives in space, then, were calculated from the following expressions:

$$\left[\frac{\delta T}{\delta z}\right]_i = 3a_i z^2 + 2b_i z + c_i \qquad (15)$$

$$\left[\frac{\delta^2 T}{\delta z^2}\right]_i = 6a_i z + 2b_i \qquad (16)$$

The cubic spline model of T(z) preserved the continuity of the first and second derivatives throughout the space domain. The time derivative of temperature was expressed with a finite difference approximation, for which (i) is the depth index:

$$\frac{\delta T}{\delta t} = \frac{T_i(t + \Delta t) - T_i(t)}{\Delta t} \qquad (17)$$

BOUNDARY AND INITIAL CONDITIONS

The solution of a one-dimensional parabolic differential equation such as equation 4 on the domain $0 < z < 95$ requires the specification of the initial condition, $T(z, t = 0)$, and two boundary conditions, at $z = 0$ and $z = 95$. The initial condition was specified with the measured soil temperatures at $t = 0$. The surface boundary condition was described as a Dirichlet boundary:

$$T(z = 0, t) = T_0(t) \qquad (18)$$

for which $T_0(t)$ was defined by measured soil temperatures at the soil surface, taken at 15-min intervals throughout the test. Intermediate values of $T_0(t)$ were represented by linear interpolation of adjacent 15-min measurements. The lower boundary condition was described as a Dirichlet boundary:

$$T(z = 95, t) = T(z = 95, t = 0) \qquad (19)$$

which is consistent with the documented experimental observation that the temperature at a sufficiently deep soil layer is time-invariant (Campbell, 1985).

METHODS AND MATERIALS

SITE DESCRIPTION

The study was performed at the Texas A&M University Farm, 11 km west-southwest of College Station, Texas, between 15 March and 16 April 1990. The Texas A&M University Farm is in the 100-yr flood plain of the Brazos River, a region consisting primarily of cattle rangeland and cotton farmland. Typical soils in the area are Norwood silt loams, Norwood silty clay loams, Weswood silt loams, and Miller clays, on 0 to 1% slopes.

The data was collected in a lysimeter 133 cm in diameter and 133 cm in depth. The soil in the lysimeter was a Weswood silt loam (fine-silty, mixed, thermic family of fluventic Ustochrepts). The soil surface was protected from precipitation throughout the study.

EQUIPMENT

Soil temperatures were measured using the copper-constantan (type T) thermocouple. Thermocouples were mounted on a wooden rod at 0, 2, 4, 7,12,19, 28, 39, 55, 75, and 95 cm, using the thermocouple junction at 95 cm as the reference junction (J0), as shown in figure 1. Soil temperatures (relative to the soil temperature at 95 cm) were measured at 900 s (15 min) intervals throughout the duration of the study.

Soil moisture measurements were made from 5 cm to 95 cm (at 10-cm intervals) on days 1, 4, 5, and 11 of the study
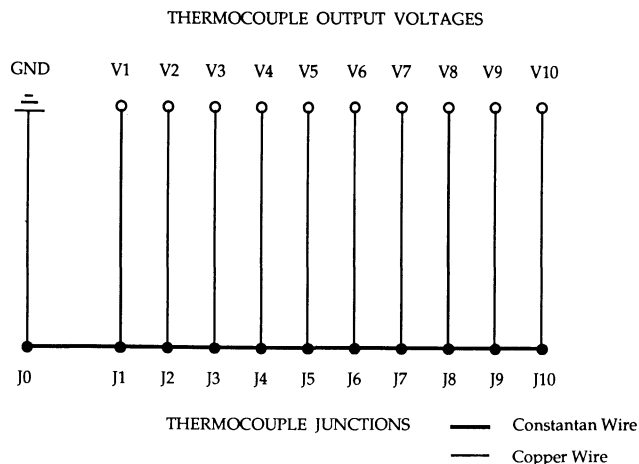

Figure 1–Schematic diagram of the thermocouple circuit.

using a neutron probe (Troxler Laboratories, model 3221). Average soil bulk density was determined in the laboratory using the standard paraffin-coated aggregate method, using seven soil samples taken at different depths within the soil profile. Soil bulk density data are shown in the next section, "Results and Discussion."

FOUR REGRESSION PROCEDURES

The procedures used to estimate the soil thermal characteristics are four variations of a regression approach proposed by Lettau (1971). In Lettau's method, equation 5 is represented with a multilinear regression model in which the two spatial derivatives of on the right-hand side of equation 5 are the independent variables, the time derivative on the left-hand side of equation 5 is the dependent variable, and the parameters α and β are the linear estimators.

Table 1 gives a description of the four variations of Lettau's regression approach evaluated in this study. Variation 1 is identical to Lettau's method, using the entire diurnal temperature cycle as the database for a two-parameter regression procedure. Variation 2 assumes that the soil thermal conductivity is independent of depth, resulting in a one-parameter linear regression. Variations 3 and 4 divide the diurnal temperature cycle into its heating and cooling components and perform regression analyses on the two smaller datasets.

RESULTS AND DISCUSSION

SOIL VOLUMETRIC HEAT CAPACITY

The soil moisture profiles measured on days 1, 4, 5, and 11 of the study are shown in Table 2. The migration of soil

TABLE 1. Description of four variations of
Lettau's regression approach

Variation	Description
1	Two-parameter regression, full diurnal cycles
2	One-parameter regression assuming, $\beta = 0$, full diurnal cycles
3	Two-parameter regression, heating cycle data only ($\delta T / \delta t > 0$)
4	Two-parameter regression, cooling cycle data only ($\delta T / \delta t < 0$)

TABLE 2. Volumetric soil moisture profiles from neutron probe measurements

Depth (cm)	Day 1	Day 4	Day 5	Day 11	Average
5.0	0.001	0.001	0.004	0.001	0.002
15.0	0.068	0.062	0.060	0.065	0.064
25.0	0.152	0.150	0.149	0.154	0.151
35.0	0.231	0.229	0.232	0.228	0.230
45.0	0.285	0.282	0.281	0.286	0.284
55.0	0.300	0.298	0.296	0.295	0.297
65.0	0.279	0.281	0.281	0.282	0.281
75.0	0.289	0.293	0.295	0.295	0.293
85.0	0.293	0.298	0.296	0.297	0.296
95.0	0.321	0.326	0.323	0.325	0.324

Figure 3–Estimates of α from variation 1 of Lettau's regression technique.

moisture over time was assumed to be negligible throughout the study, and the average of the four soil moisture profiles was used for the estimation of C_p.

The average bulk density of the soil in the lysimeter was determined from natural soil peds taken from the soil profile using the standard paraffin-clod method. The resulting average bulk density was 1.53 g/cm^3, which is consistent with published values for similar soils (Colwell, 1983). The sample standard deviation was 0.05 (n = 7) for the bulk density measurements.

Figure 2 shows the soil volumetric heat capacity as determined from bulk density and soil moisture measurements. The field data were fit ($r^2 = 0.98$) with a third-order polynomial for ease in interpolating at the thermocouple depths.
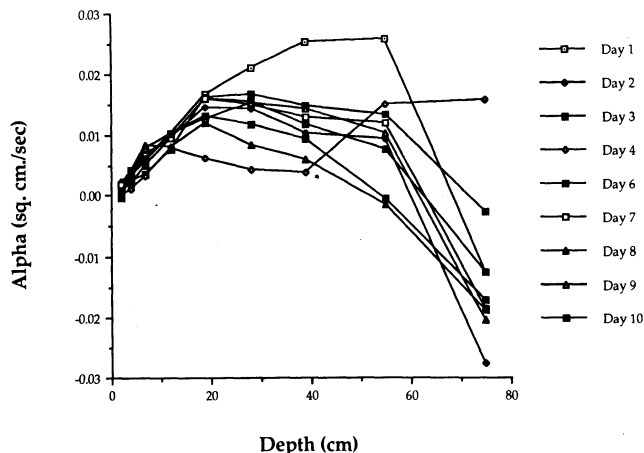
SOIL THERMAL DIFFUSIVITY

Estimates of the soil thermal diffusivity were made using the four variations of Lettau's multiple regression procedure. Figures 3 through 6 show the estimated values of α at each depth between 2 and 75 cm.

The increase in the variability of the estimates of α is primarily due to the decreased resolution in the temperature measurements at the lower depths. Below 39 cm, the

diurnal temperature variation was so slight that the analog/digital converter was often unable to resolve small temperature changes over the 900 s time interval; consequently, at the lower depths, many of the $\delta T/\delta t$ estimates took on a value of zero, causing the matrix equation from the regression analysis to approach singularity.

Other possible sources of erratic behavior of the diffusivity estimates involve the violation of one or more of the fundamental assumptions made with the least-squares regression procedure. The four assumptions, along with the terms commonly used to describe them (where applicable), are listed below:

- The regression model is linear; that is, the independent variables are not correlated with one another. (*Multicollinearity* describes the condition in which this assumption is violated.)
- All values of the dependent variable are independent of one another. (*Autocorrelation* describes the condition in which this assumption is violated.)
- The values of the dependent variable are normally distributed.

Figure 2–Variation of soil volumetric heat capacity with depth.
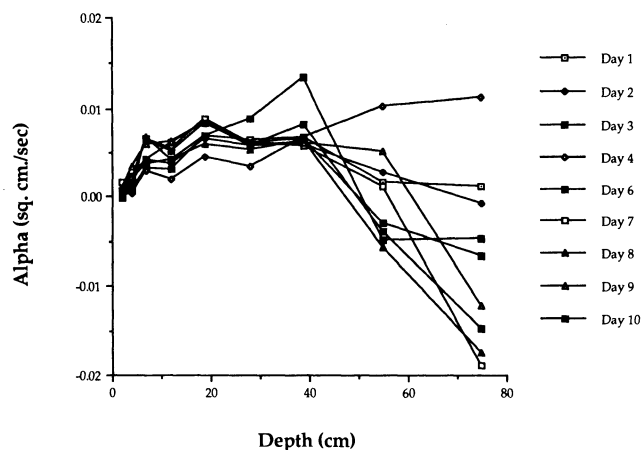
Figure 4–Estimates of α from variation 2 of Lettau's regression technique.
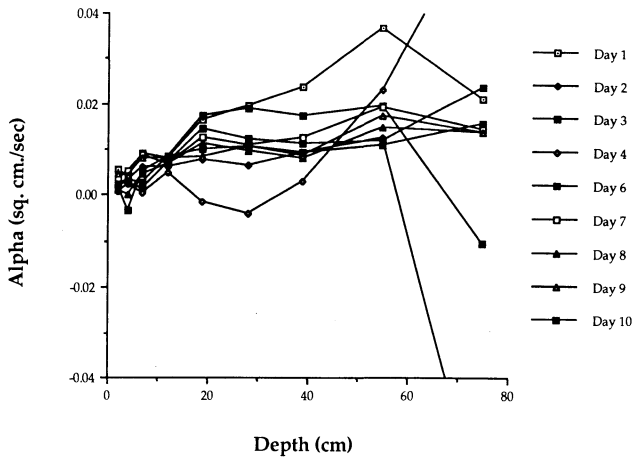
Figure 5–Estimates of α from variation 3 of Lettau's regression technique.

- The variance of the dependent variable is the same for all values of the independent variables. (When this condition is satisfied, the data set is said to be *homoscedastic*.)

The independent variables in equation 5, the first and second spatial derivatives of temperature, are closely related to one another, making the regression model inherently *multicollinear*. In simple terms, that means that the regression model is "unable to separate out the effect of each individual variable" (Hoshmand, 1988) on the dependent variable, $\delta T/\delta t$. Consequently, each regression coefficient will reflect not only the influence of its corresponding independent variable, but also the influence of the other (presumably unrelated) independent variables.

Hoshmand (1988) also states that *autocorrelation* is often observed when time series data are used in regression analysis. Such is the case with the regression procedure used in this study. Figure 7, a plot of residuals as a function of time from a two-parameter regression performed on data at 7 cm on day 7, shows an obvious time-dependence of the residual, and is an example of a graph which suggests the presence of autocorrelation. In this case, the time-interdependence of one or more independent variables is contributing to the model error.
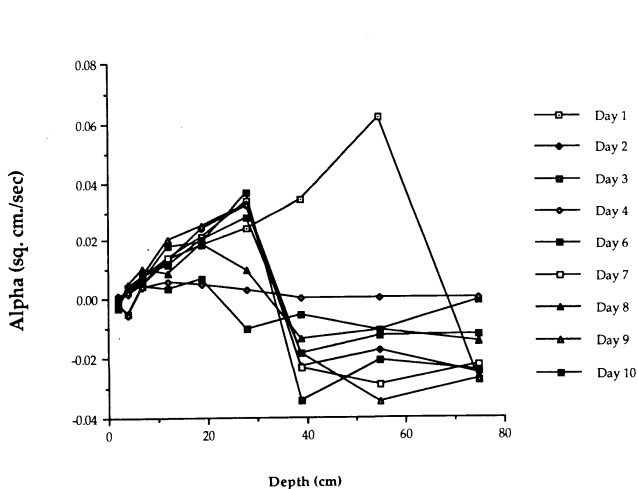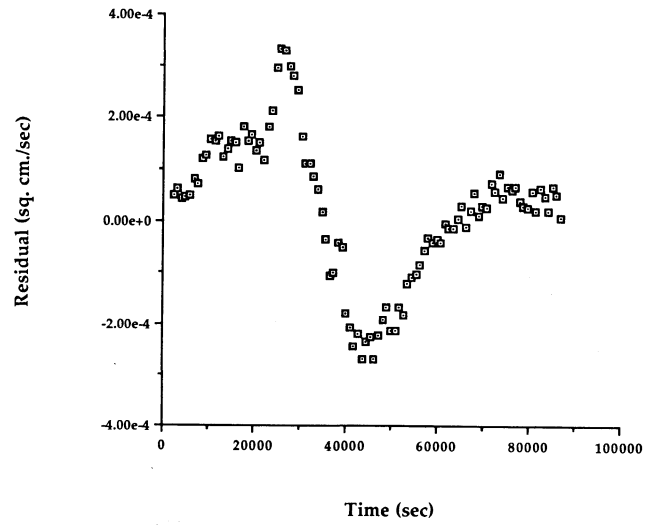

Figure 7–Time dependence of the residual from the regression procedure at 7 cm, day 7.

In order to simplify the evaluation of the four options, the daily estimates for α from each regression approach were averaged, yielding the summary in figure 8. It is evident from figures 5 and 8 that variation 3 gives more erratic results than any of the other three variations at all depths. The extreme and unpredictable behavior of variation 3 at the upper depths is due to the relatively small size of the database generated by selecting only those ordered triples for which $\delta T/\delta t > 0$; while a full diurnal regression with $\Delta t = 900$ s generated 96 data points, a heating-cycle regression at the upper depths with the same time interval generated between 30 and 40 data points, depending upon the shape of the surface temperature wave. (Heating-cycle fractions of such diurnal waves as might be encountered on hot, sunny days with low humidity may contain 30% or fewer of the diurnal data points.) Such a limitation would be remedied, of course, by decreasing the time interval between temperature measurements. For the purposes of this study, however, the predictions of the heating-cycle regression were deemed unreliable.
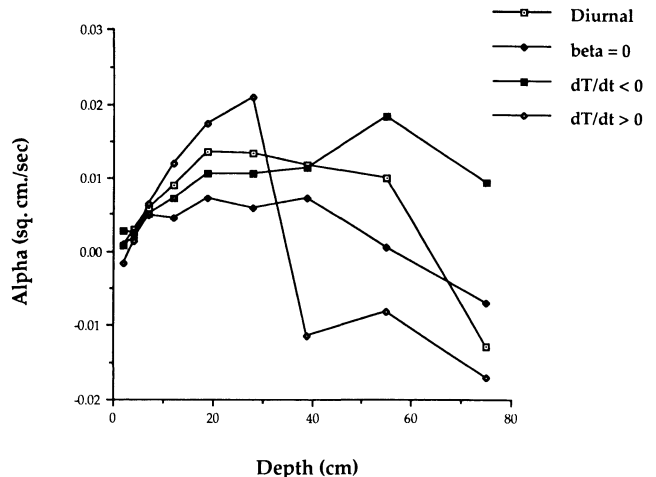

Figure 6–Estimates of α from variation 4 of Lettau's regression technique.

Figure 8–A summary of the estimates of α from the four regression procedures.
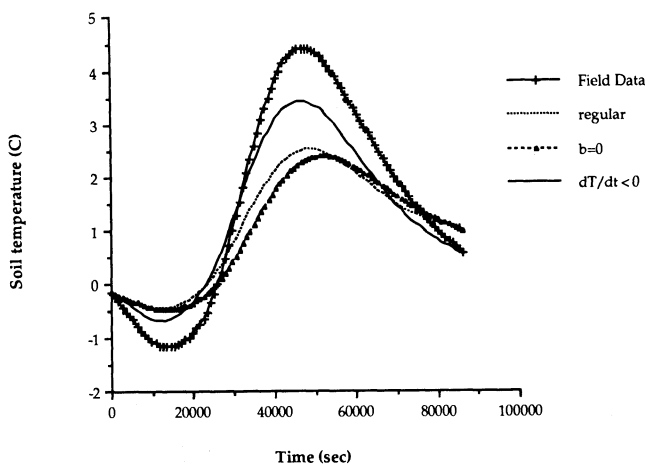
Figure 9–Soil temperature at 12 cm, as predicted by the finite difference model on day 7.
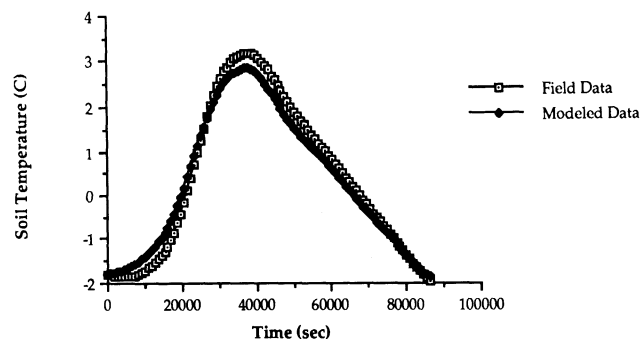

Figure 10–Measured and modeled temperatures at 12 cm, day 1.

modeled temperatures at 19 cm for days 7 and 8. This diffusivity function, which consistently overestimated the thermal transfer between soil layers, was determined to be a suitable upper boundary for a "solution envelope" in which the true diffusivity function would be expected.

Evaluation of the remaining three regression options was based upon the agreement between field temperatures and temperatures predicted by the finite-difference model. Figure 9 shows that the modeled temperatures using the diffusivity and conductivity functions estimated by the cooling-cycle regression (variation 4) most accurately reproduce field measurements, which is to be expected since the latent heat fluxes, for which the model does not account, are small during the cooling phase. The one-parameter regression (variation 2) reproduced field conditions least accurately. Average values for the soil thermal conductivity, calculated as a product of the soil thermal diffusivity (α, estimated from the cooling-cycle regression) and the volumetric heat capacity (C_p, interpolated from field measurements shown in fig. 2), are shown in Table 3.

Figures 10 and 11 show the measured and modeled temperatures at 12 cm on days 1 and 3 using the average diffusivity function from the cooling-cycle regressions in the numerical model. The agreement in both cases was good; however, the amplitudes of the modeled temperature waves were consistently smaller than those of the field temperatures, indicating that the numerical model tended to underestimate the transfer of thermal energy between soil layers. This indicated that the actual field diffusivities were probably higher than those used in the numerical model.

The numerical model was then run with the diffusivity function estimated on day 1 by the cooling-cycle regression. Figures 12 and 13 show the measured and

SUMMARY AND CONCLUSIONS

A method for *in situ* determination of the soil thermal characteristics for nonhomogeneous moisture conditions was presented. Soil volumetric heat capacity was determined from the average soil bulk density and soil moisture profiles using a weighted-average technique proposed by deVries (1963) and simplified by Campbell (1985). Four variations of a multiple regression technique proposed by Lettau (1971) for estimating the soil thermal diffusivity were evaluated. Field temperature data were compared with temperatures predicted by a finite difference model of the expanded heat equation to determine which variation produced the best estimates of α. The upper and lower boundaries were described by Dirichlet boundary conditions (time-variant at the surface, constant-temperature at the lower boundary).

In all cases, variability in estimates of the regression coefficients increased with depth due to the decreased resolution of the temperature measurements; 39 cm appeared to be the practical limit for all of the four variations of Lettau's regression technique. Consequently, comparisons among the four based upon estimates of thermal diffusivity below 39 cm were deemed inconclusive. Above 39 cm, however, the application of Lettau's technique using only temperature data from the cooling-cycle ($\delta T/\delta t < 0$) portion of the diurnal temperature
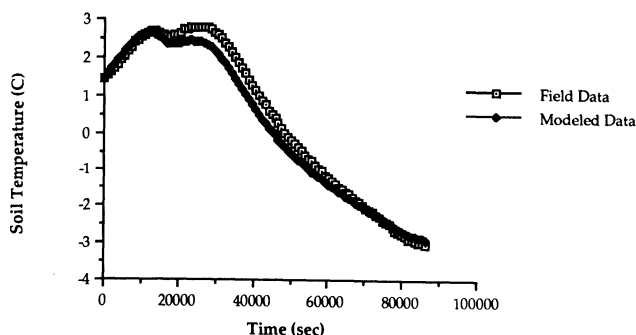
TABLE 3. Summary of estimated soil thermal properties using the cooling-cycle regression

Depth (cm)	C_p (J/cm^{3}C)	α (cm^2/sec)	λ (W/cmC)
2	1.151	0.0027	0.0031
4	1.257	0.0024	0.0030
7	1.405	0.0051	0.0072
12	1.628	0.0073	0.0118
19	1.891	0.0107	0.0202
28	2.154	0.0106	0.0228
39	2.379	0.0115	0.0274
55	2.559	0.0184	0.0471
75	2.638	0.0096	0.0253

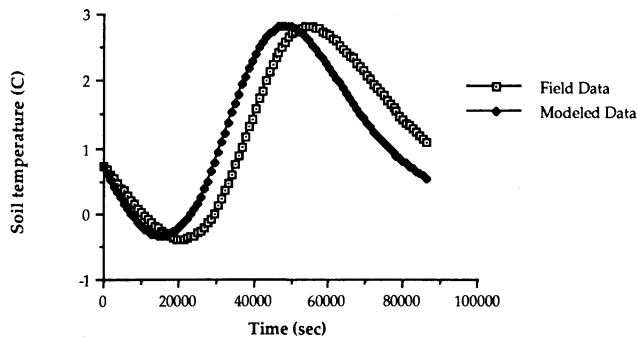Figure 11–Measured and modeled temperatures at 12 cm, day 3.

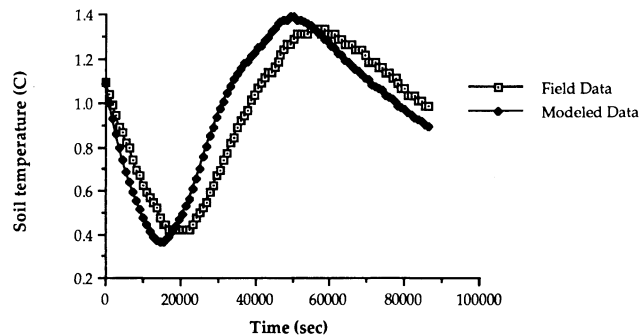**Figure 12–Measured and modeled temperatures at 19 cm, day 7.**

Figure 13–Measured and modeled temperatures at 19 cm, day 8.

wave was shown to generate the best results. There are at least two apparent reasons for that result:

- The physical model used to describe the process of thermal transfer within a soil-air system did not account for the transfer of latent heat through moisture flux, especially vapor flux; in essence, the model assumes zero vapor flux, which would be most nearly true during the cooling cycle at the surface. Therefore, the use of only cooling-cycle data removes the data which vapor fluxes would affect the most.

- The presence of higher-order (than diurnal) harmonics directly affected the accuracy of a numerical procedure which discretizes the domain. Finite-difference discretization in time obscured important short-term temperature variations which tended to arise most prominently during the heating cycle. In addition, the curvature of the time-temperature relationship tended to be less during the cooling cycle than during the heating cycle; consequently, the cooling cycle would be most suited to the finite-difference method of estimating $\delta T/\delta t$.

While the primary *predictive* value of the regression approach seems to have been affirmed, the statistical shortcomings of the approach must not be ignored, especially the violation of fundamental assumptions for a regression model. Since the terms $\delta T/\delta z$ and $\delta^2 T/\delta z^2$ are correlated by the derivative operation, the treatment of $\delta T/\delta z$ and $\delta^2 T/\delta z^2$ as independent variables in a regression procedure is statistically invalid. Also, the raw data from which the predictors arise are tainted by serial correlation; that condition, however, might be remedied through the use of autoregressive techniques. The true value of the regression model discussed in this article is limited to the prediction of the thermal characteristics, and no conclusions with respect to causality, confidence intervals, or other statistical inferences should be made.

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