Comparison of six algorithms to determine the soil apparent thermal diffusivity at a site in the Loess Plateau of China

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Abstract

Soil apparent thermal diffusivity is a crucial physical parameter that affects soil temperature. Six prevalent algorithms to calculate soil apparent thermal diffusivity are inter-compared by using soil temperature data collected at the depths of 0.05 m and 0.10 m at a bare site in the China Loess Plateau from DOY 201 through DOY 207 in 2005. Five of the six algorithms (i.e., Amplitude, Phase, Arctangent, Logarithm, and Harmonic or HM algorithms) are developed from the traditional one-dimensional heat conduction equation. The other algorithm is based on the one-dimensional heat conduction-convection equation which considers the vertical heterogeneity of thermal diffusivity in soil and couples thermal conduction and convection processes (hereinafter referred to as the Conduction-convection algorithm). To assess these six algorithms, we (1) calculate the soil apparent thermal diffusivities by using each of the algorithms, (2) use the soil apparent thermal diffusivities to predict soil temperature at the 0.10 m depth, and (3) compare the estimated soil temperature against direct measurements. Results show that (1) HM algorithm gives the most reliable estimates among the traditional five algorithms; and (2) generally, the Conduction-convection algorithm provides the second best estimates. Among all of the algorithms, the HM algorithm has the best description of the upper boundary temperature with time, but it only includes conduction heat transfer in the soil. Compared to the HM algorithm, the Conduction-convection algorithm has a less accurate description of the upper boundary temperature, but by accounting for the vertical gradient of soil diffusivity and the water flux density it includes more physics in the soil heat transfer process. The Conduction-convection algorithm has potential application within land surface models, but future effort should be made to combine the HM and Conduction-convection algorithms in order to make use of the advantages

of each.

1. Introduction

Soil temperature plays an important role in land surface processes, and it is critical in energy balance applications such as land surface modeling, numerical weather forecasting, and climate prediction (Holmes et al., 2008). It is especially true for the soil surface. Accurate prediction of soil surface temperature requires a realistic understanding of the soil thermal properties, i.e., volumetric heat capacity (C_g, J m^{-3} K^{-1}), thermal conductivity (λ, W m^{-1} K^{-1}), , and thermal diffusivity ($k = \lambda / C_g$, m^2 s^{-1}). The volumetric heat capacity C_g can be estimated as follows (De Vries, 1963),

$$C_g = (1-\theta_s)C_s + \theta C_w, \quad (1)$$

where θ is the volumetric water content, θ_s is the saturated value of θ, and C_s and C_w are the volumetric heat capacities of dry soil and water respectively. If C_g is known, only thermal conductivity, λ, or thermal diffusivity, k, must be determined to characterize the thermal properties of a soil (Passerat et al., 1996). k is of primary importance in determining soil temperature propagation (Zhang and Osterkamp, 1995). Thermal diffusivity is based solely upon conduction heat transfer. However, in soils, both conduction and convection heat transfer occur simultaneously to impact soil temperature change. Often a single parameter conduction-alone model is used to describe soil temperature changes. Since conduction and convection must be accounted for by a single parameter, the parameter must be broader than conduction alone. The parameter, often referred to as the soil thermal diffusivity, is more precisely the soil apparent thermal diffusivity, because it accounts for conduction and convection heat transfer processes that affect soil temperature change. Several algorithms have been proposed to estimate soil apparent thermal diffusivity. Most of the algorithms are based on solutions of the one-dimensional conduction heat transfer equation. Lettau (1971) calculated the apparent thermal diffusivity as a function of depth below the soil surface. In order to utilize this algorithm, measurements of soil temperature with time are required at the soil surface and at several subsurface depths. However, the lack of soil temperature data at several subsurface depths often limits the utility of this algorithm (Horton et al., 1983). Assuming that the apparent thermal diffusivity is independent of depth, and considering that temperature at the upper boundary is well described by a sinusoidal function, the analytical solution of the one-dimensional heat conduction equation can be used to estimate apparent k. Based on this solution, the apparent thermal diffusivity can be estimated by the Amplitude algorithm and Phase algorithm. Errors due to the assumption of single sinusoidal temperature wave at the soil surface can be reduced by using a Fourier series to accurately describe the diurnal variation in surface soil temperature (Van Wijk, 1963). In this way, the apparent thermal diffusivity is estimated by the Arctangent algorithm (Nerpin and Chudnovskii, 1967) with two harmonics. It was shown by Seemann (1979) that, in analogy to the Arctangent algorithm, the apparent thermal diffusivity can also be calculated by the Logarithmic algorithm. These two algorithms are analogous to the Amplitude algorithm and Phase algorithm but take advantage of greater number of temperature observations to approximate a potentially nonsinusoidal behavior (Horton et al., 1983). However, a two-harmonic function cannot describe the surface temperature very well, and a series of harmonics for the upper boundary offers advantages. Based on this boundary, the solution of the one-dimensional heat conduction equation is developed from the assumption of a sinusoidal function. According to the solution, the apparent thermal diffusivity can be selected to minimize the sum of squared differences between the calculated and measured soil temperature values (Horton et al., 1983). And it can also be estimated from an iteration process by fitting the amplitude and phase of soil temperature at one depth (Heusinkveld et al., 2004). All algorithms mentioned above are based on solutions of the one-dimensional conduction heat equation and constant diffusivity, and thus apply to uniform soils only. In fact, soil heat transfer is caused by a combination of conduction and intra-porous liquid and vapor convection (Passerat et al., 1996). Verhoef et al.(1996) described the course of topsoil thermal conductivity, diffusivity, and heat capacity during two measurement campaigns, conducted in semi-arid areas—the EFEDA-I experiment and HAPEX-Sahel. In the derivation of apparent thermal diffusivity five methods (the Amplitude, Phase, Arctangent, Logarithmic and Harmonic equation) were compared. Gao et al. (2003) pointed out that soil temperature changes in response to both conduction and convection processes, where convection was understood as 'vertical heat transfer caused by the vertical movement of liquid water in the soil'. They solved analytically the equation for one-dimensional conduction-convection, and derived a simple algorithm to accurately estimate soil thermal diffusivity.

Few efforts have been made to quantitatively test the various k algorithms by using an identical soil temperature data set. The land-air interaction over the Loess Plateau located in mid-western China affects the weather and climate in northwest China. A realistic description of soil temperature helps better understanding the land-air interaction over the Loess Plateau however few attempts have been made to determine the Loess Plateau soil thermal parameters for soil temperature algorithms. The measurements of soil temperature and soil water content during the LOess Plateau land surface process field EXperiment (LOPEX) in 2005 provided us an opportunity to evaluate the k algorithms for use on Loess Plateau soil. In order to improve the accurate knowledge of the soil apparent thermal diffusivity in this area, the objective of this paper is to compare six algorithms for determination of the soil apparent thermal diffusivity by using the direct measurements of soil temperature restricted to the upper 0.1 m of soil.

2. Theoretical considerations

Previous algorithms to calculate soil apparent thermal diffusivity k are listed in Table 1.

2.1. Classical thermal conduction equation for soil temperature

Conduction heat transfer in a one-dimensional isotropic medium is described by

$$C_g \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}(\lambda \frac{\partial T}{\partial z}), \qquad (2)$$

where T is the soil temperature (K), t the time (s), z the depth (m), C_g the volumetric heat capacity (J m^{-3} K^{-1}), and λ the thermal conductivity (W m^{-1} K^{-1}). Assuming that a soil is vertically homogeneous, in this case that C_g and λ are independent of depth, provides

$$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2}, \qquad (3)$$

where k for soil is referred to as the apparent thermal diffusivity The following five algorithms based on the solution of Eq. (3) have been used to estimate k.

2.1.1. Amplitude Algorithm

Given the surface boundary condition:

$$T\Big|_{z=0} = \overline{T} + A\sin(\omega t + \Phi), \quad (t \geq 0), \qquad (4)$$

where $\overline{T}$ is the mean soil surface temperature, A is the amplitude of the diurnal soil surface temperature wave, and ω is the angular velocity of the Earth's rotation and $\omega = 2\pi / P$ (rad s^{-1}) with P representing the period of the diurnal cycle. The soil temperature (T) at a depth z can be calculated via

$$T(z,t) = \overline{T} + A\exp(-z/d)\sin(\omega t - z/d + \Phi), \qquad (5)$$

here $d = \sqrt{2k/\omega}$ is the damping depth of the diurnal temperature wave.

Soil temperature measured at two different depths (z_1 and z_2) are often assumed to be approximated by a sinusoidal function when estimating k. The sinusoidal functions are given by

$$T\Big|_{z=z_1} = \overline{T_1} + A_1 \sin(\omega t + \Phi_1), \qquad (6)$$

$$\text{and } T\Big|_{z=z_2} = \overline{T_2} + A_2 \sin(\omega t + \Phi_2), \tag{7}$$

where A_1 (A_2), Φ_1 (Φ_2) and $\overline{T_1}$ ($\overline{T_2}$) are the amplitude, phase and mean soil temperature at the depth z_1 (z_2). $\overline{T_1}$ ($\overline{T_2}$) is the arithmetical average of the daytime maximum soil temperature and the nighttime minimum soil temperature; and A_1 (A_2) is half of the difference between the daytime maximum value and the nighttime minimum value for soil depth of z_1 (z_2); and Φ_1 (Φ_2) is the initial phase of soil temperature at depth z_1 (z_2), obtained by using the best fit algorithm (Horton et al., 1983). Then the apparent thermal diffusivity k is determined by the Amplitude algorithm

$$k = \frac{\omega(z_1 - z_2)^2}{2\ln(A_1/A_2)^2}. \tag{8}$$

2.1.2. Phase Algorithm

If the time interval between the measured occurrences of maximum soil temperature at the depths of z_1 and z_2 is $\Delta t = t_2 - t_1$, the Phase algorithm stemming from Eq. (4) is (Horton et al., 1983)

$$k = \frac{\omega(z_1 - z_2)^2}{2(\Phi_1 - \Phi_2)^2}. \tag{9}$$

2.1.3. Arctangent Algorithm

Soil surface temperature can be described by a Fourier series:

$$T = \overline{T} + \sum_{i=1}^{n}[a_i \sin(i\omega t) + b_i \cos(i\omega t)], \tag{10}$$

where n is the number of harmonics, and a_i and b_i are the amplitudes. Setting $n = 2$, k can be calculated by the Arctangent algorithm

$$k = \frac{\omega \Delta z^2}{2\left\{\arctan\left[\frac{(T_1 - T_3)(T_2' - T_4') - (T_2 - T_4)(T_1' - T_3')}{(T_1 - T_3)(T_1' - T_3') + (T_2 - T_4)(T_2' - T_4')}\right]\right\}^2}, \tag{11}$$

where temperatures T_j and T_j' are recorded each 6 h ($j = 1,2,3, and 4$) at two different depths z_1 and z_2, respectively. The first reading is taken at 02:00 (Local time, hereinafter, referred to as

LT), then 08:00 (LT), 14:00 (LT), 20:00 (LT).

2.1.4. Logarithmic Algorithm

Using the same assumption of the Arctangent algorithm, k is expressed by

$$k = \left\{ \frac{0.0121\Delta z}{\ln\left\{\left[(T_1 - T_3)^2 + (T_2 - T_4)^2\right] / \left[(T_1' - T_3')^2 + (T_2' - T_4')^2\right]\right\}} \right\}^2 . \quad (12)$$

2.1.5. Harmonic Algorithm

Eq. (10) can also be changed into another form as

$$T = \overline{T} + \sum_{i=1}^{n} C_i \sin(i\omega t + \Phi_i), \quad (13)$$

where C_i is the amplitude of the harmonic i:

$$C_i = \sqrt{a_i^2 + b_i^2}, \quad (14)$$

and Φ_i is the phase of the harmonic i:

$$\Phi_i = \arctan(a_i / b_i). \quad (15)$$

Given the following boundary condition:

$$T\Big|_{z=0} = \overline{T} + \sum_{i=1}^{n} C_{0i} \sin(i\omega t + \Phi_{0i}), \quad (t \geq 0), \quad (16)$$

the solution of Eq. (3) is

$$T(z,t) = \overline{T} + \sum_{i=1}^{n} C_{0i} \exp(-z / d_i) \sin(i\omega t + \Phi_i - z / d_i), \quad (17)$$

where C_{0i} and Φ_{0i} are the amplitude and phase of the harmonic i for the upper depth, respectively, and $d_i = \sqrt{2k/(i\omega)}$ corresponds to the depth at which the signal is propagated during a period P/i. Based on Eq. (17), the apparent thermal diffusivity k can be determined by the Least Squares Algorithm (Horton et al., 1983). On the other hand, C_{1i} (C_{2i}) and Φ_{1i} (Φ_{2i}) at the depth of z_1 (z_2) can be obtained by the approximation of the observed data at these two depths with the harmonic curve fit. In addition, according to Eq. (17), the amplitude C_{2i} and initial phase Φ_{2i} at the depth of z_2 can be predicted from

$$C_{2i} = C_{1i} \exp(-z/d_i)\,, \tag{18}$$

and $$\Phi_{2i} = \Phi_{1i} - z/d_i\,. \tag{19}$$

After an initial guess of k, the predicted results of amplitude and initial phase are compared with the fitted ones, and the parameter is adjusted depending on the differences in amplitude and initial phase (Heusinkveld et al., 2004).

2.2. Soil temperature rate equation with vertical heterogeneity of soil thermal diffusivity coupled with thermal conduction and heat transfer by water flux

Eq. (3) assumes that k is independent of depth, however, k can vary (increase or decrease) from the surface downward in the shallow surface layer of most soils. Eq. (2) can therefore be improved as follows (Gao et al., 2008):

$$\frac{\partial T}{\partial t} = \frac{1}{C_g}\frac{\partial}{\partial z}(\lambda \frac{\partial T}{\partial z}) = \frac{\lambda}{C_g}\frac{\partial^2 T}{\partial z^2} + \frac{1}{C_g}\frac{\partial \lambda}{\partial z}\frac{\partial T}{\partial z} \approx k\frac{\partial^2 T}{\partial z^2} + \frac{\partial k}{\partial z}\frac{\partial T}{\partial z}\,. \tag{20}$$

Neglecting the vertical heterogeneity of k, Gao et al. (2003) incorporated thermal conduction and convection together as follows:

$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial z^2} - \frac{C_{\mathrm{w}}}{C_{\mathrm{s}}} w\theta \frac{\partial T}{\partial z}\,. \tag{21}$$

where w is the liquid flow rate (positive downward) and θ is the volumetric water content of the soil. C_w is the heat capacity of water. Assuming these three parameters are also independent of z for a thin soil layer in present work, $-\frac{C_{\mathrm{w}}}{C_s} w\theta$ was defined as water flux by Gao et al. (2003). Based on Eqs. (19) and (21), Gao et al. (2008) presented the following equation

$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial z^2} + W\frac{\partial T}{\partial z}\,, \tag{22}$$

where $W = \frac{\partial k}{\partial z} - \frac{C_w}{C_s} w\theta$ consisted of the vertical gradient of soil diffusivity ($\frac{\partial k}{\partial z}$) and the water flux density ($-\frac{C_w}{C_s} w\theta$).

With the boundary condition Eq. (7), the expression of the soil temperature at the depth z_1 is

$$T(z_1,t)=\overline{T_1}+A_2\exp[-\alpha(z_1-z_2)M]\sin[\omega t+\Phi_2-\alpha(z_1-z_2)N], \qquad (23)$$

where $M=\frac{\alpha}{\omega}\{W+\frac{1}{\sqrt{2}}[W^2+(W^4+\frac{4\omega^4}{\alpha^4})^{1/2}]^{1/2}\}$ and $N=\sqrt{2}(\frac{\omega}{\alpha})[W^2+(W^4+\frac{4\omega^4}{\alpha^4})^{1/2}]^{-1/2}$.

They also gave the expression of k and W

$$k=-\frac{(z_1-z_2)^2\omega\ln(A_1/A_2)}{(\Phi_1-\Phi_2)\left[(\Phi_1-\Phi_2)^2+\ln^2(A_1/A_2)\right]}; \qquad (24)$$

$$W=\frac{\omega(z_1-z_2)}{\Phi_1-\Phi_2}\left[\frac{2\ln^2(A_1/A_2)}{(\Phi_1-\Phi_2)^2+\ln^2(A_1/A_2)}-1\right]. \qquad (25)$$

We call it as Conduction-convection algorithm in this paper. Applying $W=0$ to Eq. (25) results in $\Phi_2-\Phi_1=-\ln(A_2/A_1)$ or $-\ln(A_2/A_1)=\Phi_2-\Phi_1$, then Eq. (24) reduces to be Eq. (8) or Eq. (9).

3. Field Experiments

The experiment was conducted on soil in the China Loess Plateau during an intensive observation period from DOY 197 through 241 in LOPEX in 2005. The soil measurements were collected at a bare soil site located at 106.42°E, 35.35°N at an altitude of 1592 m in Pingliang county of Gansu Province in western China.

The ground surface of this site was bare, flat and homogeneous. The soil at the site was predominantly medium loam with a high proportion of silt. The site is located within a semiarid climate zone. The maximum air temperature was 307 K and the lowest was 249 K, the annual air temperature and precipitation were 279K and 510 mm with 2425 hours of sunshine, and 170 frost-free days per year all averaged over the last 50 years (Gao et al., 2008). The bulk density was 1250 kg m^{-3}, and soil solid heat capacity was 1.40×10^6 J m^{-3} K^{-1}.

Soil temperature was measured with four TCAV averaging soil thermocouple probes (Campbell Scientific Inc., U.S.A.) at 0.05 and 0.10 m depths. The volumetric water content of the soil was measured at 0.05 and 0.10 m depths by two soil moisture reflectometers (CS615, Campbell Scientific Inc. USA). All of the sensor outputs were recorded and averaged over 10 min intervals.

4. Results

The data used in this paper were collected in a 7-day period from (DOYs 201 through 207 (i.e., 20 through 26 July), 2005. The soil temperature measured at 0.05 and 0.10 m depths changed diurnally during DOYs 203-207, as shown in Figure 1a. The amplitudes of the soil temperature decreased and the phases shifted ahead when the soil depth increased. The soil temperature at 0.05 m changed in response to intermittent cloudiness during DOYs 202 and 203. The maximum soil temperature reached 310.78 K on DOY 204, and the minimum soil temperature was 287.77 K at 0.05 m depth on DOY 203. Figure 1a also shows that the soil vertical temperature gradient reached 191.20 K m^{-1} for the soil layer from 0.05 to 0.10 m depths at 14:45 (LT) on DOY 204 at this site.

The temporal variations in volumetric soil water content at 0.05 and 0.10 m depths during the same period are shown in Figure 1b. Precipitation occurred from DOYs 199 to 201 with an amount of 15.7 mm. Since then, owing to evaporation from the bare soil surface, the soil volumetric water content was decreasing gradually at both depths from DOYs 202 through 207. Gao et al. (2008) pointed out that under evaporation conditions there is a net upward flux of water (liquid and vapor) that responds to the progressively drying surface condition. The net flux of water causes an associated net convective heat flux. The soil physics implies that the heat transfer should incorporate a vertical convective heat transfer component.

After using a 2-hour smoothing technique for soil temperature measured at the depth of 0.05 m, A_1, A_2, Φ_1, Φ_2, $\overline{T_1}$, $\overline{T_2}$, $\overline{T}$, C_i and Φ_i are obtained by using the approximation of soil temperature collected at the depths of 0.05 m and 0.10 m for each day, respectively. Smoothing reduces amplitudes, but we are concerned with A_1/A_2. The reduction in both A_1 and A_2 does not influence A_1/A_2 much. The temporal variations of k are calculated by using the Amplitude, Phase, Conduction-convection and HM algorithms (Horton et al., 1983, Heusinkveld et al., 2004, Gao et al., 2008) for the soil layer from 0.05 m to 0.10 m. Temperatures at each depth for the arbitrary times of 02:00 (LT), 08:00 (LT), 14:00 (LT), and 20:00 (LT) were used for

Arctangent algorithm and Logarithmic algorithm. Results are shown in Figure 2. The Amplitude, Arctangent, Logarithmic and HM algorithms provided relatively low values of k during this period. This is especially true for the Arctangent algorithm. The Phase algorithm and the Conduction-convection algorithm provided k values approximately twice as large as the other algorithms. The two HM algorithms provided similar values of k. The thermal diffusivity estimated by the Logarithmic algorithm changed from day to day in the drying period. The maximum, minimum and mean values of k calculated by these six algorithms are listed in Table 2. The smallest value of k is 0.6×10^{-7} m^2 s^{-1}, and it is obtained from the Arctangent algorithm on DOY 202. The maximum value is 5.47×10^{-7} m^2 s^{-1}, and it is obtained from the Phase algorithm on DOY 207. The maximum, minimum and mean values of k calculated by the Phase algorithm and by the Conduction-convection algorithm are larger than the values derived by the other algorithms. The two HM algorithms and the Amplitude algorithm provide similar estimates of the mean values of k.

5. Discussion

The variations of the apparent thermal diffusivity k obtained by the six algorithms with the volumetric soil water content θ for the 0.05 m to 0.10 m layer are shown in Figure 3. Estimates of k from five of the six algorithms change in a narrow range with θ during this drying period ($\theta < 25\%$). The exception is the Logarithmic algorithm. The values of k from the Phase algorithm and the Conduction-convection algorithm have similar trends with θ. The variations of k shown by the other four algorithms show a similar trend with θ. These results make sense because values of k from the Phase and the Conduction-convection algorithms mainly depend on $\Phi_1 - \Phi_2$, while estimates of k with the other algorithms mainly depend on the amplitude. All of the algorithms indicate that the largest value of k does not occur at the largest soil water content. Gao et al. (2008) showed that k does not monotonically increase with increasing θ. It tends to increase as dry soil begins to wet, but it approaches a constant value or even decreases as the soil continues to wet.

In the Conduction-convection algorithm, another parameter W is needed and is calculated with Eq. (25) (see values in Table 3).

The measured and modeled soil temperatures at the 0.10 m depth from DOY 201 through 207 are presented in Figure 4. It is obvious that the fitted temperature by using Arctangent, Logarithmic and the two HM algorithms gave poor approximation in the early morning of DOY 203 because the assumption of repeating surface periodic temperature is not valid between DOY 202 and 203. To better show the model outputs, we take DOY 204 as an example (see Figure 5). Overall, The Phase algorithm reasonably estimated the soil temperature phases but overestimated the amplitudes, and the amplitude algorithm reasonably estimated the soil temperature amplitudes but overestimated the phase shift. In fact, as shown in Table 4, the values of $\ln(A_1/A_2)$ are larger than $\Phi_1 - \Phi_2$ for the whole 7-day period. Using the Phase algorithm to estimate k implies forcing $\ln(A_1/A_2)$ to be equal to $\Phi_1 - \Phi_2$, which overestimates the soil temperature amplitude by about 0.74 K on average for DOYs 201 to 207. Similarly, using the Amplitude algorithm to estimate k implies that $\Phi_1 - \Phi_2$ is equal to $\ln(A_1/A_2)$, which overestimates the soil temperature phase shift by $\ln(A_1/A_2) - (\Phi_1 - \Phi_2) = 0.2397$ rad (55 minutes) on average for DOYs 201 to 207.

The Logarithmic and Arctangent algorithms require four pairs of soil temperature measurements. The modeled k values are very sensitive to the measurement time of four pairs of soil temperatures, so we have to average the calculated values of k for different selections of four pairs of soil temperatures for each day.

The two HM algorithms generated similar values of k. For most of the study days, the HM algorithm gave realistic estimations of soil temperature at the depth of 0.10 m. However, as mentioned above, it did not give a good estimation in the early morning of DOY 203 because of the invalid assumption of the repeating periodic for soil temperature. Results obtained by two HM algorithms indicate that fitting measurements of soil temperature by using the Least Squares approach directly and simultaneously determining the amplitude and initial phase of the soil temperature may provide realistic values of k. Comparison of the results obtained by the HM algorithms, Phase algorithm, Amplitude algorithm, Logarithmic algorithm and Arctangent algorithm shows that the HM algorithms gave the most accurate values of k. This conclusion agrees with those by both Horton et al. (1983) and Verhoef et al. (1996).

The Conduction-convection algorithm provided realistic daytime soil temperature values. However, it underestimated the soil temperature during the period from 18:00 (LT) to 08:00 (LT), and a noteworthy difference between the measurements and the model output occurred around 00:00 (LT) for all days in this study. A similar underestimation was also encountered by Lin (1980) and Gao et al. (2008). Our explanation is that the model always keeps W constant although the actual W may decrease to zero or even become negative during the nighttime, and also the model does not account for water phase changes that usually happen in shallow soil during the nighttime.

Scatter plots of soil temperature modeled by using the six algorithms against the measured soil temperature at the depth of 0.1 m are given in Figure 6. The results show that the HM algorithms and Conduction-convection algorithm generated larger correlation coefficients (r), than did the other algorithms. All of the regression lines had slopes of 1.

Statistical analyses are also used to examine the error of model output as follows,

$$SEE = \sqrt{\frac{\sum_{i=1}^{n}(T_m - T)^2}{n-2}}, \tag{26}$$

$$NSEE = \sqrt{\frac{\sum_{i=1}^{n}(T_m - T)^2}{\sum_{i=1}^{n} T^2}}. \tag{27}$$

Where n is the total number of data points; SEE is the standard error of the estimate; and $NSEE$ is a normalized SEE which denotes an estimate of relative uncertainty. The statistical indices SEE and $NSEE$ are presented in Table 5 for the modeled period. It is obvious that the HM algorithm has the lowest values both of SEE and $NSEE$. The Conduction-convection algorithm has the second lowest values of SEE and $NSEE$

Another comparison of the accuracies of the six algorithms is shown in Figure 7 using the empirical probability distribution functions (PDF) of difference between the modeled and measured soil temperatures at the depth of 0.10 m. The differences between the modeled and measured soil temperatures using the HM algorithm ranged between -1 K and 1 K, and most were near zero. The Conduction-convection algorithm generated the second best results.

6. Conclusions

Six algorithms for calculating soil apparent thermal diffusivity are evaluated with shallow soil measurements collected during LOPEX in 2005. The Phase algorithm and the Amplitude algorithm overestimated the phase and overestimated the amplitude of the soil temperature, respectively. Although the Arctangent algorithm and the Logarithmic algorithm only required four measures of temperature spaced equally in time at two depths, the timing of the four measures of temperature affected the values of soil apparent thermal diffusivity greatly. The HM algorithm gave a reasonable result for most days. However, the assumption of repeating periodicity for soil temperature is invalid on cloudy or rainy days. The algorithms mentioned above are based upon the one-dimensional conduction equation. The Conduction-convection algorithm which is based on the one-dimensional conduction-convection equation, provided satisfactory results for daytime temperatures, but it systematically underestimated nighttime soil temperatures. Overall, the Conduction-convection algorithm provided better results than all of the other algorithms except for the HM algorithm. Future efforts should focus on combining the HM and the Conduction-convection algorithms in order to develop an improved method that combines the advantages of each algorithm. The new method should include multiple harmonics to describe the upper boundary temperatures and include conduction and convection heat transfer processes.

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Figures:

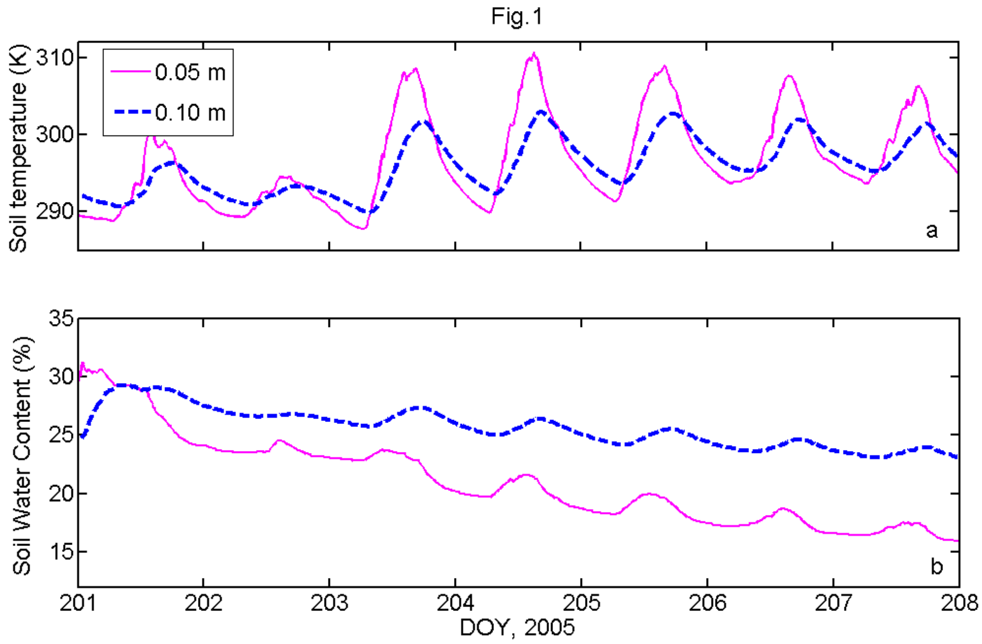

Figure 1. Temporal variations of (a) soil temperature (K) and (b) soil water content (%) measured at depths of 0.05 m and 0.10 m at a bare soil site over the Loess Plateau from DOY 201 through DOY 207, 2005.

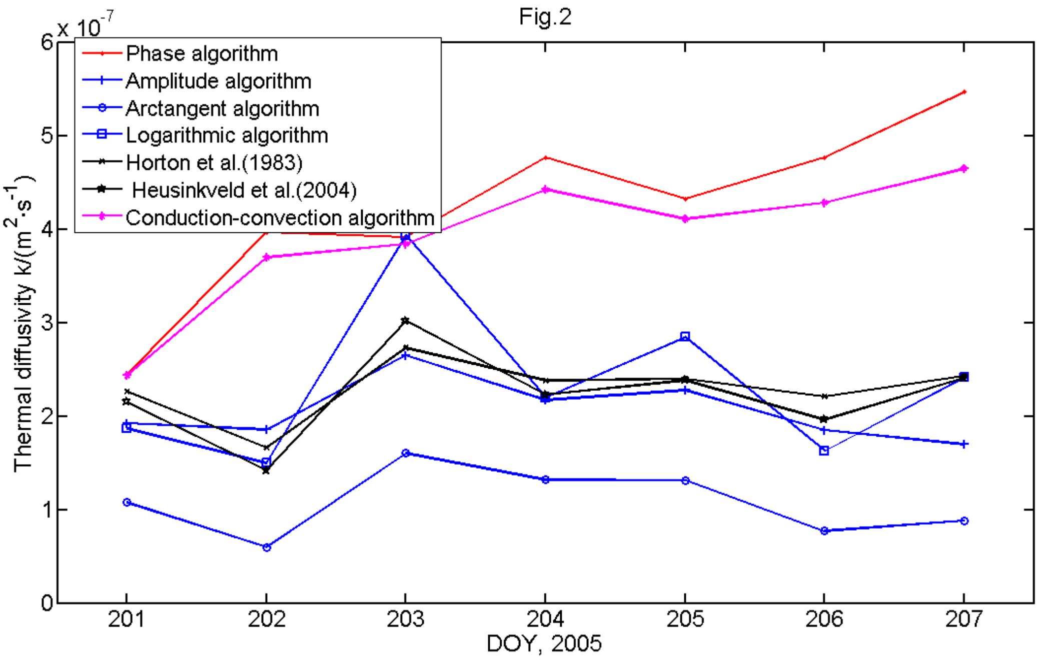

Figure 2. Temporal variation of soil apparent thermal diffusivity k (m^{-2} s^{-1}) at a bare soil site over the Loess Plateau from DOY 201 through 207, 2005.

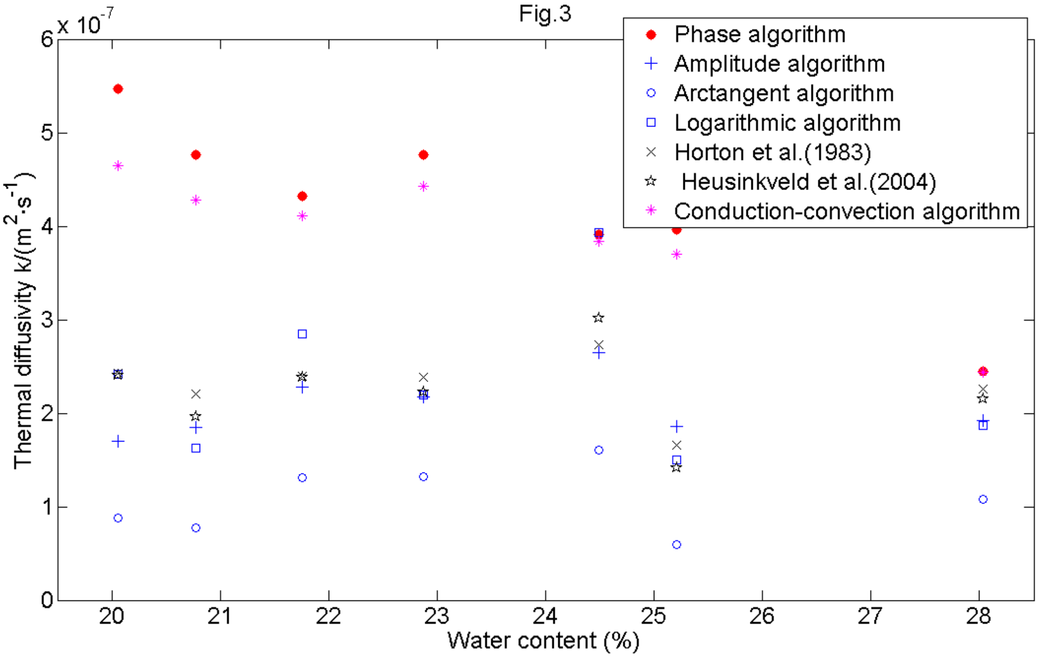

Figure 3. Variation of soil apparent thermal diffusivity k (m^2 s^{-1}) with volumetric soil water content θ (%) at a bare soil site over the Loess Plateau from DOYs 201 through 207, 2005.

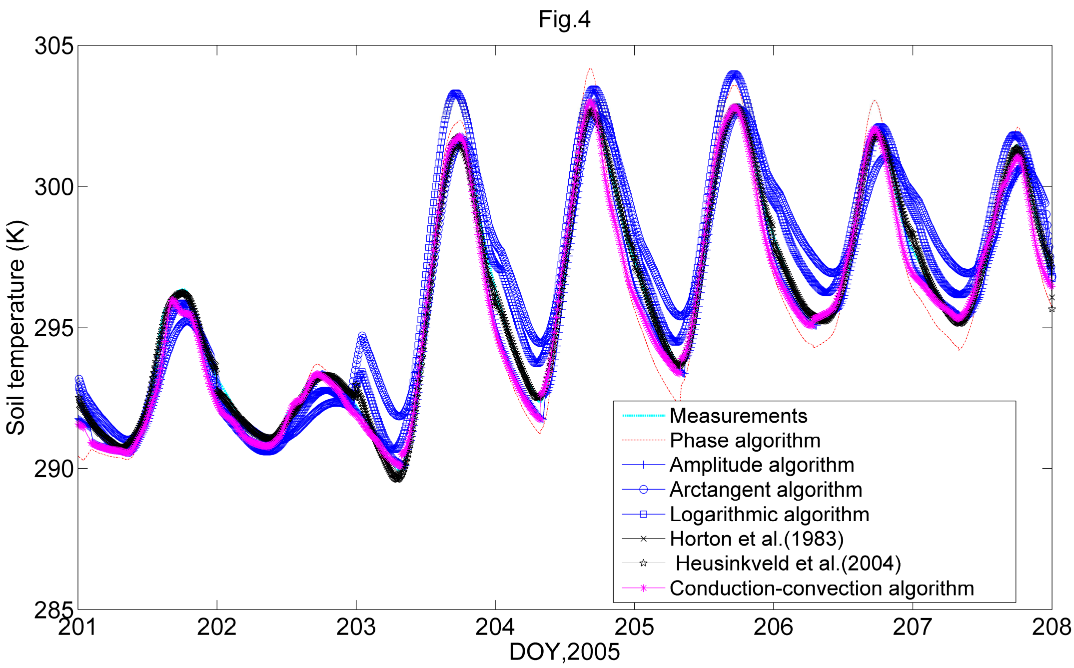

Figure 4. Comparisons of soil temperature modeled by using Phase algorithm, Amplitude algorithm, Arctangent algorithm, Logarithmic algorithm, algorithm by Horton et al.(1983), algorithm by Heusinkveld et al.(2004), and Conduction-convection algorithm, against measurements of soil temperature at 0.10 m depth at a bare soil site over the Loess Plateau from DOYs 201 through 207, 2005.

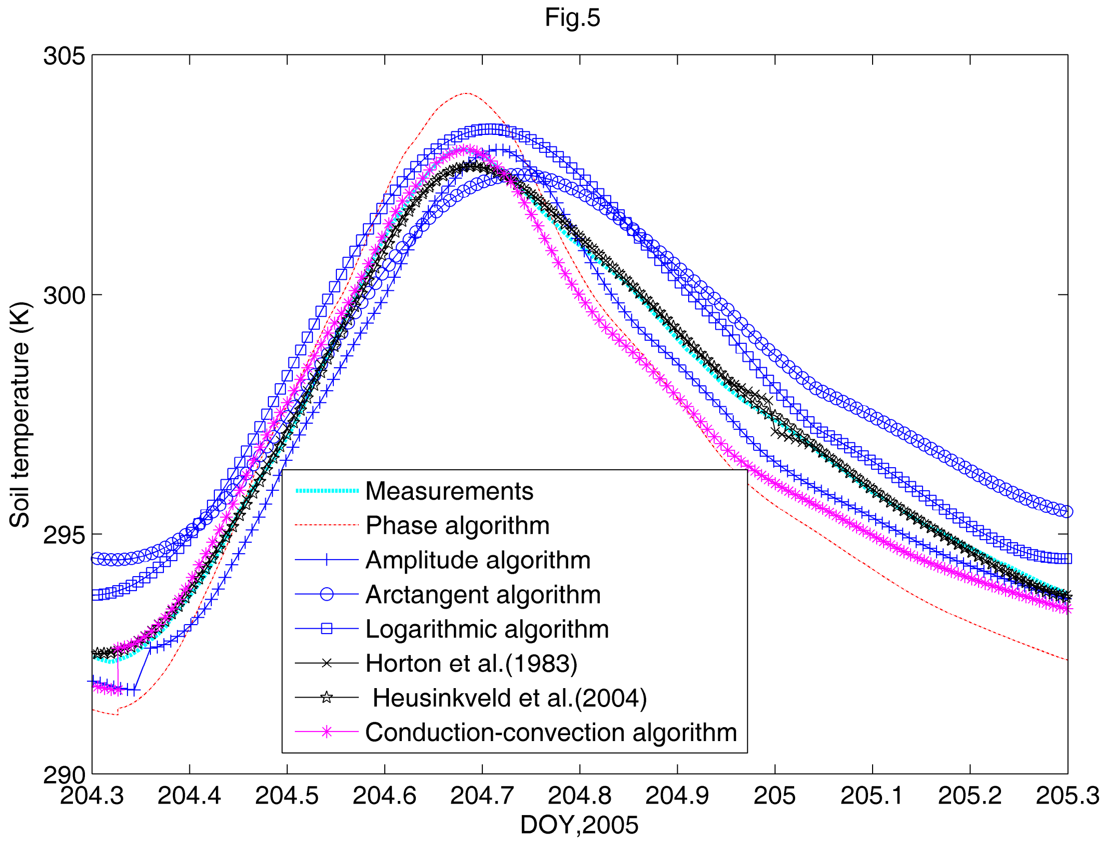

Figure 5. Comparisons of soil temperature modeled by using Phase algorithm, Amplitude algorithm, Arctangent algorithm, Logarithmic algorithm, algorithm by Horton et al.(1983), algorithm by Heusinkveld et al.(2004), and Conduction-convection algorithm, against measurements of soil temperature at 0.10 m depth at a bare soil site over the Loess Plateau on DOY 204, 2005.

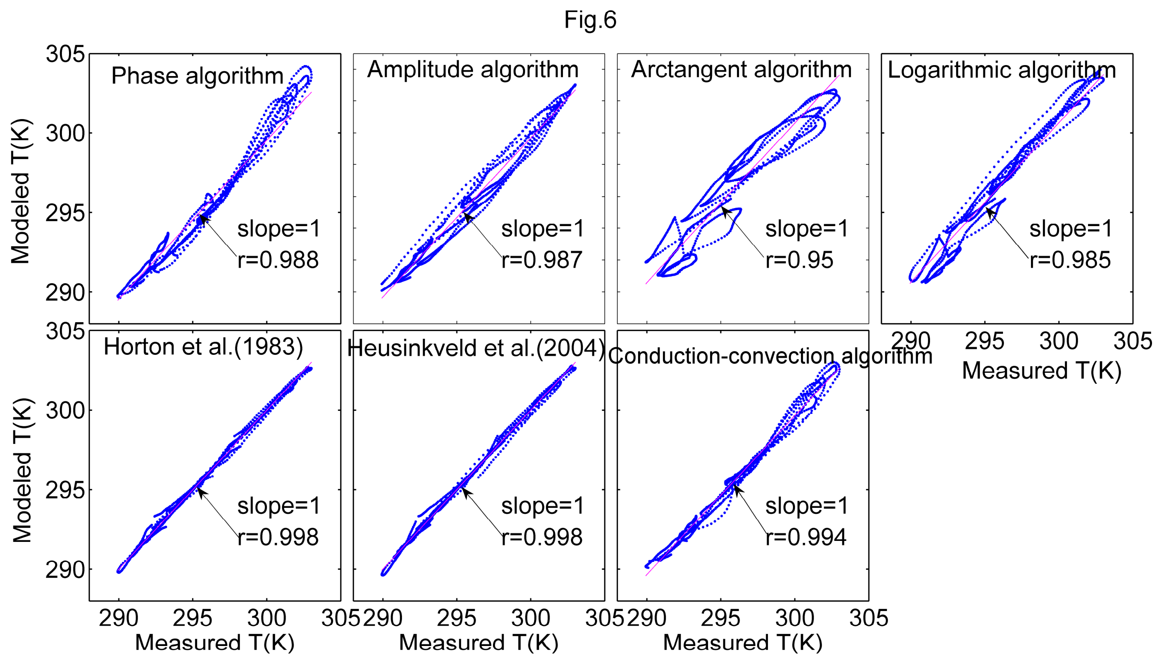

Figure 6. Scatter plots of the temperature modeled by using Phase algorithm, Amplitude algorithm, Arctangent algorithm, Logarithmic algorithm, Horton et al.(1983), Heusinkveld et al.(2004), and Conduction-convection algorithm for the soil depth of 0.10 m against the soil temperature at 0.10 m depth from DOY 201 to DOY 207, 2005.

Fig.7

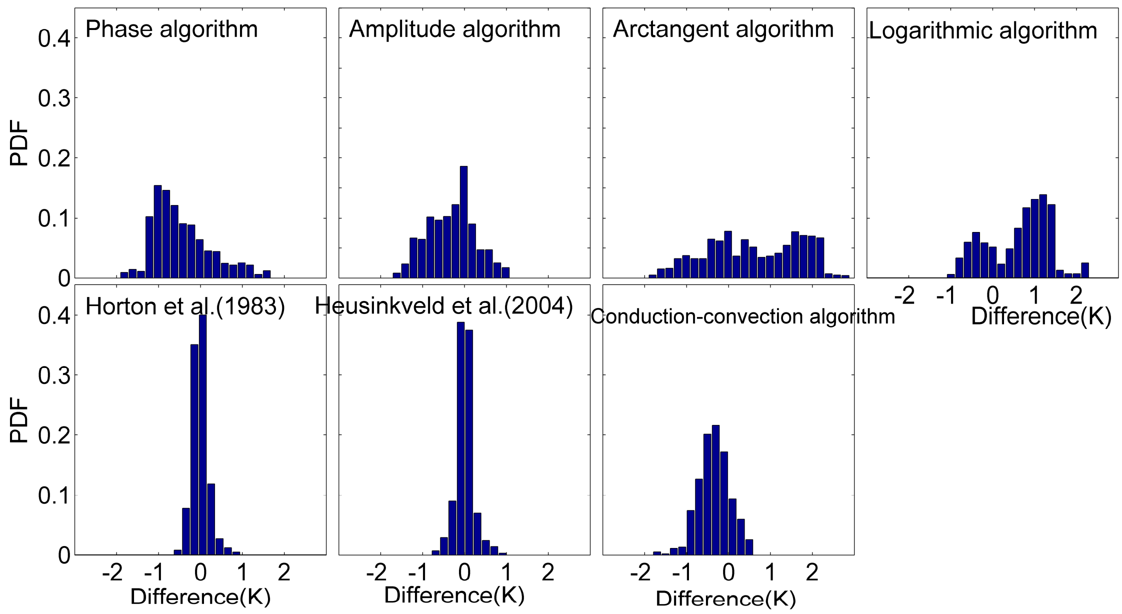

Figure 7. Empirical probability distribution function, PDF, of subtraction between the temperature modeled by using the Phase algorithm, Amplitude algorithm, Arctangent algorithm, Logarithmic algorithm, Horton et al.(1983), Heusinkveld et al.(2004), and Conduction-convection algorithm for the soil layer ranging from 0.05 m to 0.10 m with the soil temperature at 0.10 m depth from DOY 201 to DOY 207, 2005.

Tables

Table 1. See another independent file named as “Table 1.doc”

Table 2 The maximums, minimums and mean values of k calculated by six algorithms for the layer of 0.05-0.10m on the Loess Plateau from DOY 201 to DOY 207, 2005.

Name	Max ($k \times 10^7$)	Min ($k \times 10^7$)	Mean ($k \times 10^7$)
Phase algorithm	5.47	2.45	4.24
Amplitude algorithm	2.65	1.69	2.06
Arctangent algorithm	1.60	0.60	1.07
Logarithmic algorithm	3.93	1.50	2.34
HM(Horton et al.,1983)	3.02	1.42	2.22

HM(Heusinkveld et al., 2004)	2.73	1.66	2.30
Conduction-convection algorithm	4.65	2.43	3.92

Table 3 The values of W calculated by Conduction-convection algorithm for the layer of 0.05-0.10m on the Loess Plateau from DOY 201 to DOY 207, 2005.

DOY	W ($\times 10^7$ m s^{-1})
201	0.722
202	2.755
203	1.454
204	3.112
205	2.453
206	3.669
207	4.696

Table 4 The values of the phase shift and the logarithm of amplitude ratio of soil temperature obtained by using one sine function approximation algorithm at the 0.05m and 0.10m depths on the Loess Plateau from DOY 201 to DOY 207, 2005.

DOY	$\Phi_1 - \Phi_2$	$\ln(A_1/A_2)$
201	0.6008	0.6875
202	0.4788	0.7001
203	0.4819	0.5858
204	0.4367	0.6468
205	0.4587	0.6316
206	0.4367	0.7008
207	0.4078	0.7323

Table 5 Computed Standard Error of the Estimate (SEE) and Normalized Standard Error of the Estimate (NSEE) of soil temperature at 0.10m depth on the Loess Plateau from DOY 201 to DOY 207, 2005.

Name	SEE	NSEE
Phase algorithm	0.8288	0.0028
Amplitude algorithm	0.6481	0.0022
Arctangent algorithm	1.2693	0.0043

Logarithmic algorithm	0.9796	0.0033
HM(Horton et al., 1983)	0.1963	0.0006
HM(Heusinkveld et al., 2004)	0.2132	0.0007
Conduction-convection algorithm	0.5091	0.0017