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Soil Heat Storage Measurements in Energy Balance Studies

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Abstract

Energy balance studies require knowledge of the heat flux at the soil surface. This flux is determined by summing the heat flux at a reference depth (z_r) some centimeters below the surface and the rate of change of heat storage in the soil above z_r The rate of change of heat storage, or *heat storage* for short (ΔS), is calculated from soil volumetric heat capacity (C) and temperature. The objectives of this study were to determine how choices regarding z_r, C measurements, and ΔS calculations all affect the accuracy of ΔS data. Heat transfer theory and data from three field sites were used toward these ends. In some studies, shallow reference depths have been used and ΔS neglected. Our results indicate that when z_r is sufficiently deep to permit accurate heat flux measurements, ΔS is too large to neglect. Three methods for determining C were evaluated: soil sampling, the ThetaProbe soil moisture sensor, and heat pulse sensors. When C was determined using all three methods simultaneously, the estimates agreed to within 6% on average; however, the temporal variability of C was best recorded with the automated heat pulse sensors. Three approaches for calculating ΔS were also tested. The common approach of letting C vary in time but neglecting its time derivative caused errors when soil water content was changing. These errors exceeded 200 W m^{-2} in some cases. The simple approach of assuming a constant C performed similarly. We introduce a third approach that accounts for the time derivative of C and yields the most accurate ΔS data.

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ABSTRACT

Energy balance studies require knowledge of the heat flux at the soil surface. This flux is determined by summing the heat flux at a reference depth (z_r) some centimeters below the surface and the rate of change of heat storage in the soil above z_r. The rate of change of heat storage, or *heat storage* for short (ΔS), is calculated from soil volumetric heat capacity (C) and temperature. The objectives of this study were to determine how choices regarding z_r, C measurements, and ΔS calculations all affect the accuracy of ΔS data. Heat transfer theory and data from three field sites were used toward these ends. In some studies, shallow reference depths have been used and ΔS neglected. Our results indicate that when z_r is sufficiently deep to permit accurate heat flux measurements, ΔS is too large to neglect. Three methods for determining C were evaluated: soil sampling, the Theta-Probe soil moisture sensor, and heat pulse sensors. When C was determined using all three methods simultaneously, the estimates agreed to within 6% on average; however, the temporal variability of C was best recorded with the automated heat pulse sensors. Three approaches for calculating ΔS were also tested. The common approach of letting C vary in time but neglecting its time derivative caused errors when soil water content was changing. These errors exceeded 200 W m^{-2} in some cases. The simple approach of assuming a constant C performed similarly. We introduce a third approach that accounts for the time derivative of C and yields the most accurate ΔS data.

MEASUREMENTS of the surface energy balance provide valuable scientific information. These measurements contribute greatly to our understanding of the dynamic transfers of water, energy, and trace gases at the Earth's surface. Energy balance studies in terrestrial ecosystems require measurements of soil heat flux. Typically, soil heat flux is measured at a reference depth a few centimeters below the soil surface rather than directly at the surface (Ochsner et al., 2006). The heat flux at the surface is then calculated as the sum of the flux at the reference depth and the rate of change of heat storage above the reference depth (ΔS).

The heat storage is estimated based on the soil volumetric heat capacity, C, and temperature, T. The formal relationship is

$$\Delta S = \int_0^{z_r} \frac{\partial}{\partial t} [C(T - T_0)]dz \qquad [1]$$

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where z_r is the reference depth, t is time, and T_0 is an arbitrarily assigned reference temperature. In this study, we chose $T_0 = 0°C$. Inspection of Eq. [1] shows that four steps must be taken to determine soil heat storage. First, the reference depth must be chosen. Second, soil temperature must be recorded. Third, soil heat capacity must be determined. Fourth, heat storage must be calculated using some approximation of Eq. [1]. Approximation is necessary because soil temperature and heat capacity data are usually discontinuous in depth and time.

A review of published energy balance studies shows considerable variability in the chosen reference depths. Recent studies have used reference depths ranging from 1 mm (Heusinkveld et al., 2004) to 10 cm (Tanaka et al., 2003). Shallow reference depths are sometimes chosen with the intent of minimizing the integral in Eq. [1] so that heat storage can be neglected (Baldocchi et al., 2000; da Rocha et al., 2004; Heusinkveld et al., 2004; Wilson et al., 2000). A shallow reference depth, however, may create the potential for large errors in soil heat flux measurements (Buchan, 1989). Neglecting heat storage above the reference depth may also lead to significant errors in soil heat flux (Mayocchi and Bristow, 1995). The first objective of this study was to illustrate the magnitude of soil heat storage above the reference depth and to offer some considerations for choosing an appropriate reference depth.

Methods for making the soil temperature measurements required in Eq. [1] are not evaluated in this study. The interested reader is referred to the chapter by McInnes (2002) for a good discussion of methods for measuring soil temperature. Most data acquisition systems used in energy balance studies can readily support high-frequency, long-term soil temperature measurements.

In contrast, soil heat capacity data are more difficult to obtain. One method that has been used for many years is the estimation of heat capacity from water content and bulk density determined by soil sampling (Payero et al., 2005; Sauer et al., 1998; Twine et al., 2000). More commonly now, heat capacity is estimated based on data from soil water content sensors (Giambelluca et al., 2003; Hunt et al., 2002; Kellner, 2001; Ogée et al., 2001; Tanaka et al., 2003). Soil sampling is still required to determine bulk density in this method. A third approach is to measure heat capacity directly using heat pulse sensors (Bremer and Ham, 1999; Ham and Knapp, 1998). The second objective of this study was to compare these three methods for determining soil heat capacity.

To precisely evaluate Eq. [1] would require heat capacity and temperature data that were continuous in depth and time. Such data are rarely if ever available. In practice, approximations to Eq. [1] must be used to accommodate data that are discontinuous. Massman (1993) carefully evaluated some of the errors in heat storage that arise from using such approximations. He

showed that using a depth-averaged heat capacity and temperature measurements at two depths led to errors of 3 to 10% in the estimated soil heat flux. He also proposed some weighting factors for the temperature data to reduce these errors. The analysis was based on the assumption that heat capacity did not vary with time. Of course, soil heat capacity does vary with time, especially near the surface. The effects of these temporal variations need to be examined.

The third objective of this study was to evaluate the merits of three different approximations to Eq. [1]. The primary distinguishing feature between the approximations is the manner in which temporal variations in heat capacity are represented. The first and most common approximation is to let heat capacity vary with time, but to assume that the time derivative of heat capacity is negligible (Ogée et al., 2001). The second and simplest approximation is to assume a constant value for heat capacity (Triggs et al., 2004). The third approximation, which we introduce, includes temporal variations in heat capacity and also includes the time derivative of heat capacity.

In summary, the objectives of this study were to determine how choices regarding the reference depth, heat capacity measurements, and approximations to Eq. [1] all affect the accuracy of soil heat storage data. Toward these ends, basic soil heat transfer theory and data from three field sites will be used.

MATERIALS AND METHODS

Field Sites

We performed field experiments to measure soil heat storage under a bare soil surface, a soybean [*Glycine max* (L.) Merr.] canopy, and a corn (*Zea mays* L.) canopy. During the summer of 2001, we measured heat storage in the surface soil from 0 to 6 cm in a small plot of bare soil. The site was located in central Iowa, a few kilometers northwest of Ames. The soils at the site belong to the Canisteo–Clarion–Nicollet association (Typic Haplaquolls–Typic Hapludolls–Aquic Hapludolls). Measurements began on 3 July and continued until 9 August. The average daily maximum value of solar radiation was 828 W m^{-2} during the measurement period.

During the summer of 2002, we measured heat storage in the surface soil from 0 to 6 cm deep in adjacent fields of soybean and corn. The fields were located in central Iowa, a few kilometers south of Kelley. The soils at these sites belong to the Clarion–Nicollet–Webster association (Typic Hapludolls–Aquic Hapludolls–Typic Haplaquolls). Measurements at both sites began on 18 June and continued until 29 July at the soybean site and 14 August at the corn site. The soybean was planted in east–west rows with 30-cm row spacing, and the corn was planted in east–west rows with 76-cm row spacing. The average daily maximum value of net radiation was 634 W m^{-2} at the soybean site and 616 W m^{-2} at the corn site during the measurement period. At the corn site, the ground cover was estimated at 40% on 17 June and reached 95% by 2 July. At the soybean site, the ground cover was estimated at 10% on 17 June and reached 55% by 9 July. Near-complete ground cover at the soybean site was reached around 18 July.

Soil Properties

Some basic physical properties for the 0- to 6-cm soil layer at the three sites are listed in Table 1. These data include

Table 1. Particle-size distribution, organic matter content, and bulk density for the soils from the three field sites.

Site	Particle size			Organic matter content	Bulk density
	Sand	Silt	Clay		
		%		g kg^{-1}	Mg m^{-3}
Bare soil	32	25	43	65	1.13
Soybean	54	21	25	31	1.26
Corn	45	23	32	54	1.14

the particle-size distributions, organic matter contents, and bulk densities. The particle-size distributions were determined by the hydrometer method (Gee and Or, 2002). The USDA textural class for the soil at the bare soil site was clay, while the soils at the soybean and corn sites were classified as sandy clay loams. The total C content of the soils was determined by dry combustion (Nelson and Sommers, 1996), and organic matter content was estimated based on the total C content. For determining bulk density, 7.6-cm-diameter by 7.6-cm-high soil cores were collected at the bare soil site. The cores were collected with a Uhland core sampler (Uhland, 1949). Bulk density was determined using three such cores representing the 0- to 7.6-cm soil layer. At the soybean and corn sites, samples were obtained by tapping a thin-walled ring (7.3 cm in diameter and 3.7 cm high) into the soil by hand using a small block of wood and a hammer. Then the ring and the soil it contained were excavated with a putty knife. Separate samples were taken for the 0- to 3.7-cm and 3.7- to 7.4-cm soil layers. At the soybean site, four of these small samples were collected, and at the corn site, eight samples were collected. The samples were taken to the lab, weighed, oven dried at 105°C for 24 h, and reweighed to determine bulk density.

Heat Capacity Measurements

Soil Sampling

The first method for estimating heat capacity was based on soil sampling to determine mass water content. Soil cores 1.9 cm in diameter were collected and divided into 0- to 3-, 3- to 5-, and 5- to 7-cm depth increments. Composite samples for each layer were stored in moisture cans. The samples were taken to the laboratory, weighed, oven dried at 105°C for 24 h, and reweighed to determine mass water content. Samples for water content were obtained with an average of 1.6 d between samples for the bare soil site and 2.3 d between samples for the soybean and corn sites. Bulk density was determined by soil sampling as described above.

Once water content and bulk density were determined, heat capacity was calculated as the weighted sum of the heat capacities of the various soil constituents (Kluitenberg, 2002). Values for the specific heat of the soil mineral and organic fractions were taken from de Vries (1963) specific heat values. Heat capacity data from this soil sampling method will be identified by C_{SS}.

Soil Moisture Sensor

The second method for estimating heat capacity relied on measurements of volumetric water content using an electromagnetic impedance sensor. At each site, measurements of the average volumetric water content in the top 6 cm of soil were made using a ThetaProbe (Delta-T Devices Ltd., Cambridge, England). The ThetaProbe infers water content based on the transmission and reflection of a 100-MHz sinusoidal electromagnetic signal along four 6-cm-long stainless steel rods embedded in the soil. The ThetaProbe was vertically inserted into the soil during site visits to determine water content;

however, automated in situ measurements are possible with the ThetaProbe and most other electromagnetic sensors.

At the bare soil site, water content was estimated using the ThetaProbe from 20 July to 6 August, with an average of 1.6 d between measurements. At the soybean site, ThetaProbe measurements were taken from 3 to 29 July, with an average interval of 2.4 d. At the corn site, measurements were taken from 3 July to 14 August, with an average interval of 2.3 d. The manufacturer's mineral soil calibration was used for all three sites. The resulting volumetric water content data were used along with measured bulk density and organic matter values and the de Vries (1963) specific heat values to obtain the ThetaProbe heat capacity estimates (C_{TP}).

Heat Pulse Sensors

Direct measurement using heat pulse sensors was the third method that we evaluated for determining heat capacity. To measure heat capacity using a heat pulse sensor, a brief pulse of heat is introduced by the sensor's small heating element (3–4 cm long, ~1-mm diam.) and the resulting temperature increase 6 mm away at the sensing needle is measured and recorded. The maximum temperature increase is inversely proportional to the heat capacity (Campbell et al., 1991).

Two different designs of heat pulse sensors were used to measure heat capacity. In 2001, six three-needle heat pulse sensors based on the design of Ren et al. (1999) were installed at the bare soil site. The sensors were installed horizontally at 2, 4, and 6 cm below the soil surface with two sensors at each depth. The center needle was the heating needle and was positioned at the desired depth with temperature sensing needles 6 mm above and below. In 2002, eight two-needle heat pulse sensors (Thermal Logic, Pullman, WA) based on the design of Campbell et al. (1991) were installed at both the soybean site and the corn site. These sensors were installed horizontally at 1.5 and 4.5 cm below the soil surface, with four sensors at each depth. The two-needle sensors were positioned with the heating and sensing needles in the same horizontal plane, and the needle spacing was 6 mm.

The measurement systems for the heat pulse sensors consisted of a datalogger (21x, Campbell Scientific, Logan, UT), a thermocouple multiplexer (AM25T, Campbell Scientific), a multiplexer for the heating circuits (AM416, Campbell Scientific), a reference resistor for measuring the current through the heaters, a relay for switching the current, and a deep-cycle 12-V battery. At the bare soil site, an AM416 multiplexer was used for the thermocouples in place of the AM25T multiplexer. A thermistor (107, Campbell Scientific) was mounted on the center bridge of the multiplexer to provide reference temperature measurements.

The three-needle sensors were heated for 10 s and the two-needle sensors were heated for 8 s. The measured voltage drop across the reference resistor was used to determine the heating power. The temperature of each sensor was measured before heating and one time per second for 75 s after the initiation of heating. For each sensor, the maximum temperature increase and the heating power were used to calculate the heat capacity (C_{HP}). Heat pulse measurements were performed every hour.

The needle spacing for each heat pulse sensor was calibrated by recording measurements of heating power and temperature rise with the sensor immersed in water stabilized with agar (6 g L^{-1}) to prevent convection. An in situ matching point calibration procedure was also used. All the heat capacity measurements for each sensor were shifted up or down by a constant value to make the heat capacity measurement from the sensor equal the heat capacity estimate based on soil sampling on the date of the first available soil sampling data. This matching point calibration procedure reduces the variability between sensors (Ochsner et al., 2003).

Heat Storage Calculations

Approximations to Eq. [1] are typically developed by first splitting the integral into two terms:

$$\Delta S = \int_0^{z_r} C \frac{\partial T}{\partial t} dz + \int_0^{z_r} (T - T_0) \frac{\partial C}{\partial t} dz \qquad [2]$$

The second term on the right-hand side of Eq. [2] is neglected in the most common approximation. The neglect of this term is necessary when the time derivative of heat capacity, $\partial C/\partial t$, is unknown, i.e., when determinations of heat capacity are infrequent. Dropping this term and discretizing Eq. [2] gives

$$\Delta S \left(\frac{t_j + t_{j-1}}{2} \right) = \sum_{i=1}^{N} C_{i,j-1} \frac{T_{i,j} - T_{i,j-1}}{t_j - t_{j-1}} (z_i - z_{i-1}) \quad [3]$$

where i and j are index variables for depth layers and time steps, respectively.

Equation [3] splits the soil into N layers and uses the assumptions that heat capacity and temperature are constant with depth inside each layer and that $\partial C/\partial t$ is negligible.

The second approximation is a further simplification in which a depth-averaged constant value is used for the heat capacity. Equation [3] then becomes

$$\Delta S \left(\frac{t_j + t_{j-1}}{2} \right) = C \sum_{i=1}^{N} \frac{T_{i,j} - T_{i,j-1}}{t_j - t_{j-1}} (z_i - z_{i-1}) \quad [4]$$

The constant heat capacity value can be calculated from estimated values of the typical water content and bulk density for the soil.

When heat capacity is determined frequently relative to the time scale of its temporal variability, a more accurate approximation of Eq. [1] can be used. In that case we approximate Eq. [1] by

$$\Delta S \left(\frac{t_j + t_{j-1}}{2} \right) = \sum_{i=1}^{N} \frac{C_{i,j}(T_{i,j} - T_0) - C_{i,j-1}(T_{i,j-1} - T_0)}{t_j - t_{j-1}}$$
$$\times (z_i - z_{i-1}) \qquad [5]$$

Equation [5] is more general than Eq. [3] because no assumption regarding the magnitude of $\partial C/\partial t$ is necessary. We are not aware of any previous use of this approximation in the context of energy balance studies.

For all sites and methods, soil temperature was measured with Cu-constantan thermocouples at 2, 4, and 6 cm below the surface, and the reference depth was 6 cm. Applying the Massman (1993) corrections at the bare soil site where gradients of heat capacity and temperature were steepest changed the heat storage estimates by only about ±2 W m^{-2}. Given the degree of uncertainty in assigning the correction factors, we chose not to use these corrections.

We chose hourly time steps to calculate heat storage. At smaller time steps, temperature measurement errors have larger effects. For example, in a 6-cm soil layer with $C = 2 \times 10^6$ MJ m^{-3} K^{-1}, a 0.1°C error in the measured change in temperature leads to a 13 W m^{-2} error in storage for a 15-min time step but only a 3 W m^{-2} error for a 1-h time step. For hours when heat capacity was not measured (there were intervals of days between measurements of C_{SS} and C_{TP}), we used the most recently measured value of heat capacity that was available. Table 2 provides further details on how Eq. [3] through [5] were applied.

Table 2. Soil layers and measurement depths used in calculating the rate of change of heat storage from 0 to 6 cm by three different methods based on measured soil temperature (T) and heat capacity (C).

Method	Layer no.	Upper boundary	Lower boundary	Depth of T measurement	Depth of C measurement
			cm		
Soil sampling	1	0	3	2	0–3
	2	3	5	4	3–5
	3	5	7†	6	5–7
ThetaProbe	1	0	6	2, 4‡	0–6
Heat pulse§	1	0	3	2	1.5
	2	3	6	4	4.5

† In Eq. [3], a multiplier of 0.5 was included for Layer 3.
‡ The arithmetic mean of the temperature measurements at 2 and 4 cm was used.
§ Layers, boundaries, and T measurement depths for the heat pulse method at the bare soil site were the same as for the soil sampling method, and C was measured at 2, 4, and 6 cm.

RESULTS AND DISCUSSION

Reference Depth and the Magnitude of Soil Heat Storage

Soil heat storage, and the errors caused by its neglect, increase as the reference depth increases. Soil heat storage is manifest in two ways: first, in the decreasing amplitude of the heat flux wave with depth, and second, in the time lag of the wave with depth. A simple approximation for the reduction in the amplitude of the diurnal heat flux wave as a function of reference depth is plotted in Fig. 1a (see Appendix for formula and derivation). Results are given for a range of thermal diffusivities (α) encompassing many soils. Figure 1a shows that, at a depth of 1 cm, the maximum soil heat flux is 7 to 13% less than the maximum at the surface. The discrepancy increases as the reference depth increases. At 10 cm, the maximum soil heat flux is 49 to 74% less than the surface maximum. When heat storage is neglected, soil heat flux is underestimated by these same amounts. These systematic errors in soil heat flux would contribute to overestimating available energy during the daytime in Bowen ratio studies and underestimating daytime energy balance closure in eddy covariance studies.

The shift in the timing of the estimated heat flux wave as a function of reference depth is plotted in Fig. 1b (see Appendix for f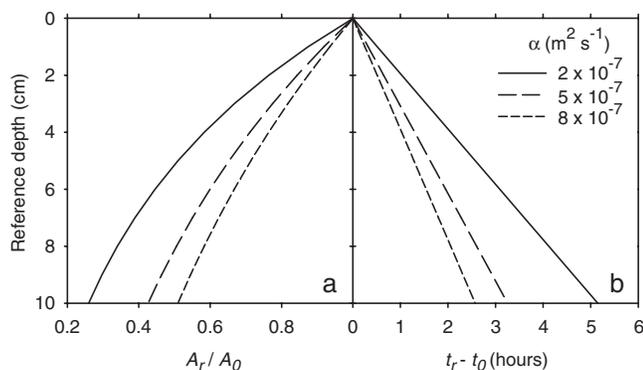ormula and derivation). At a depth of 1 cm, the peak heat flux occurs 15 to 31 min after the surface peak. Again, the discrepancy increases as reference depth increases. At 10 cm, the peak occurs 2.6 to 5.2 h after the surface peak. When heat storage is neglected, this time lag is translated to the soil heat flux data. These timing errors in estimated soil heat flux may reduce the accuracy of half hourly or hourly estimates of available energy or energy balance closure.

Data from the field sites show the magnitude of soil heat storage for a 6-cm reference depth with different levels of canopy cover (Fig. 2). The magnitude of soil heat storage increased as ground cover decreased. At the bare soil site, the absolute value of the rate of change of heat storage in the top 6 cm exceeded 70 W m^{-2} 10% of the time. At the corn site, the absolute value of heat storage only exceeded 30 W m^{-2} 7% of the time. The magnitude of soil heat storage at the soybean site was typically intermediate. Figure 2 can be viewed as showing the magnitude of the error in soil heat flux that would have been caused by neglecting storage.

Several other problems may arise with shallow heat flux measurements in addition to these errors from neglecting storage. A sensor placed immediately beneath the soil surface may impede the transfer of water (liquid and vapor) into and out of the soil, thereby altering the heat flux. Westcot and Wierenga (1974) reported
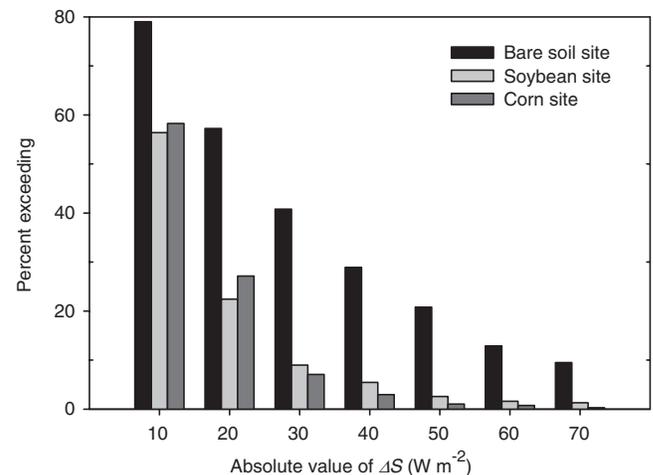

Fig. 1. (a) Ratio of the amplitude of soil heat flux at the reference depth (A_r) to the amplitude of the soil heat flux at the surface (A_0) as a function of reference depth for three values of thermal diffusivity (α); (b) difference between the time of maximum heat flux at the reference depth (t_r) and time of maximum heat flux at the soil surface (t_0) as a function of reference depth.

Fig. 2. Absolute values for the rate of change of heat storage (ΔS) in the top 6 cm of soil as determined using heat pulse sensors (Eq. [5]) at the bare soil, soybean, and corn sites.

that the transfer of water vapor accounted for 40 to 60% of the total heat flux in the 0- to 2-cm soil layer during periods of the day. Ochsner et al. (2006) found that impervious plastic disks 2 cm below the soil surface increased the magnitude of the soil water content and temperature gradients two- to threefold. These results suggest that heat flux plates buried at 1 cm may significantly distort and misrepresent soil heat flux. Furthermore, in energy balance studies, it is usually desirable to include energy that is consumed in evaporation below the soil surface in the latent heat flux term rather than in soil heat flux. But, any energy consumed in evaporation below the reference depth will be mistakenly included in the soil heat flux. Choosing a reference depth very near the soil surface increases the likelihood for this error, which may reach 100 W m^{-2} in extreme cases (Buchan, 1989).

In summary, neglecting heat storage will often lead to errors that are large relative to the soil heat flux. Under a dense canopy (e.g., forest) the soil heat flux may be quite small relative to the net radiation and sensible and latent heat fluxes measured above the canopy. In that case, the errors introduced by neglecting heat storage above the reference depth might be acceptable. Soil heat flux, however, is an important component of the energy balance below the canopy, a zone of great ecological interest (Ogée et al., 2001). So even under dense canopies, caution should be used when considering whether to use a shallow reference depth and neglect soil heat storage. No minimum acceptable value for the reference depth is universally applicable, but in general it should not be too shallow and soil heat storage should not be neglected. In our experience, reference depths from 5 to 10 cm produce good results.

Comparing Methods for Measuring Heat Capacity

When C_{SS}, C_{TP}, and C_{HP} were determined simultaneously, all three heat capacity estimates were similar. To compare the heat capacity measurements, the average values of heat capacity for the 0- to 6-cm soil layer were calculated using each method. The 1200 h value of C_{HP} was chosen to compare with the values of C_{SS} and C_{TP} for each day that soil samples and ThetaProbe readings were collected. The 1200 h value was chosen because the soil samples and ThetaProbe readings were usually collected around midday. The mean absolute differences listed in Table 3 indicate the extent of agreement between the three methods. The best agreement is between C_{TP} and C_{SS} at the soybean site, where the

mean absolute difference was 0.04 MJ m^{-3} K^{-1} or 2% of the mean value of heat capacity for that site. The poorest agreement was between C_{TP} and C_{HP} at the bare soil site, where the mean absolute difference was 0.15 MJ m^{-3} K^{-1} or 8% of the mean heat capacity for that site.

Linear regressions showed moderately strong relationships ($r^2 = 0.66$–0.83) between heat capacity estimates from these three methods (Table 4). Inferences regarding the slopes and intercepts of the regressions were based on the 95% confidence intervals. For all three regressions, the slopes were not significantly different from unity, and the intercepts were not significantly different from zero.

Perhaps the most notable bias was the tendency of C_{TP} to overestimate C_{HP} and C_{SS} at the bare soil site. In the clay-textured soil at the bare soil site, C_{TP} was on average 6% greater than C_{SS} or C_{HP}. This bias is not surprising since electromagnetic sensors often require special calibrations for soils with high clay content. The performance of the ThetaProbe at this site could probably be improved by developing a specific calibration for this soil.

The time series of C_{SS}, C_{TP}, and C_{HP} at each site are presented in Fig. 3 along with the time series of daily rainfall measured by tipping bucket rain gauges. These data show that rainfall events caused sudden increases in heat capacity and that these peaks were best recorded by the automated heat pulse sensors. In contrast, capturing the peaks in heat capacity by soil sampling is difficult. For example, at the soybean site, soil sampling before rainfall on 26 July and again on 29 July resulted in a 2.5-d lag between the rainfall and the increase in C_{SS}, and this lag led to a 39% underestimate of heat capacity for that period. In general, the C_{SS} and C_{TP} data show that sampling even three times per week was not frequent enough to consistently record the temporal variations in heat capacity of the near-surface soil.

Heat Storage Estimates

The heat storage estimates were not much affected by the method used for determining heat capacity. This is not surprising since the three methods we tested returned similar values for heat capacity. Table 5 presents linear regression results comparing hourly heat storage estimates based on soil sampling, ThetaProbe, and heat pulse estimates of heat capacity. For each method, heat storage was calculated using Eq. [3] to facilitate a direct comparison. The ThetaProbe data led to heat storage estimates that were 7 to 8% greater than those from soil sampling or the heat pulse method. Again, this is due primarily to overestimates of heat capacity at the bare

Table 3. Mean absolute differences in estimates of volumetric heat capacity obtained from soil sampling (C_{SS}), from Theta-Probe data (C_{TP}), and from heat pulse sensors (C_{HP}). Mean values of C_{HP} are included for comparison.

Site	Mean absolute differences			Mean value
	$\|C_{SS} - C_{HP}\|$	$\|C_{TP} - C_{HP}\|$	$\|C_{TP} - C_{SS}\|$	C_{HP}
	MJ m^{-3} K^{-1}			
Bare soil	0.07	0.15	0.14	1.80
Soybean	0.12	0.11	0.04	1.80
Corn	0.10	0.09	0.06	1.68

Table 4. Results from linear regressions of heat capacity measured by heat pulse sensors (C_{HP}), estimated by soil sampling (C_{SS}), and estimated from ThetaProbe measurements (C_{TP}).

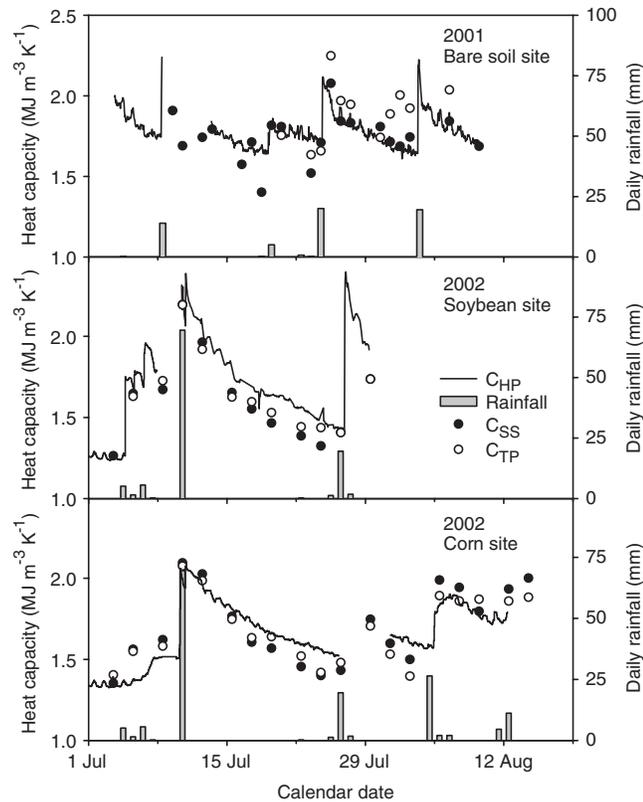| Comparison (y vs. x)	Slope	Intercept	r^2
		MJ m^{-3} K^{-1}	
C_{SS} vs. C_{HP}	0.996	−0.034	0.752
C_{TP} vs. C_{HP}	0.961	0.0625	0.658
C_{TP} vs. C_{SS}	0.923	0.158	0.831

Fig. 3. Time series of heat capacity measured by heat pulse sensors (C_{HP}), estimated by soil sampling (C_{SS}), and estimated from Theta-Probe measurements (C_{TP}) along with daily rainfall totals for the three sites.
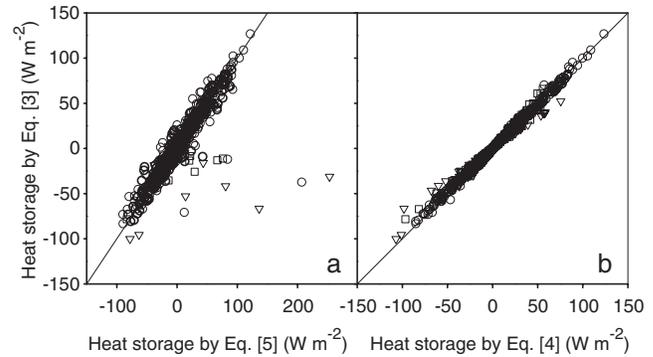

Fig. 4. Heat storage calculated using Eq. [3] vs. (a) heat storage calculated using Eq. [5], and (b) heat storage estimated by Eq. [4]. The solid lines are the 1:1 lines.

soil site by the ThetaProbe. The soil sampling method and heat pulse method produced very similar heat storage estimates when Eq. [3] was used for both. The slope of that relationship is just 2.2% below unity. All of the slopes in Table 5 are significantly different from unity, and none of the intercepts are significantly different from zero based on the 95% confidence intervals.

The heat storage estimates were more affected by the different approximations to Eq. [1] than by the method used for determining heat capacity. We used the hourly data from the heat pulse sensors at each site and calculated heat storage using Eq. [3], [4], and [5]. Figure 4a compares the results from using Eq. [3], which neglects $\partial C/\partial t$, with the results from using Eq. [5], which includes $\partial C/\partial t$. Ninety-one percent of the data fall within ±10 W m^{-2} of the 1:1 line, but there are some data points from each site that fall >80 W m^{-2} below the 1:1 line. These points correspond to sudden peaks in heat capac-

Table 5. Results from linear regressions of hourly values of rate of change of heat storage. Heat capacity was determined by soil sampling (SS), ThetaProbe (TP), and heat pulse sensors (HP). Equation [3] was used with all three methods.

Comparison (y vs. x)	Slope	Intercept	r^2
		W m^{-2}	
SS vs. HP	0.978	−0.054	0.994
TP vs. HP	1.07	0.041	0.989
TP vs. SS	1.08	0.040	0.995

ity following rainfall events when $\partial C/\partial t$ contributed significantly to the heat storage. At these times, the commonly used Eq. [3] resulted in large errors.

Figure 4b compares the results from Eq. [3] with the results from Eq. [4], which assumes a constant heat capacity for each site. In this case, the heat capacity for each site was set equal to the time-averaged value measured by the heat pulse sensors at that site. These two approximations gave very similar results. Ninety-nine percent of the data lie within ±10 W m^{-2} of the 1:1 line, with no noticeable outliers. This implies that making hourly measurements of heat capacity and then using Eq. [3] to calculate heat storage does not yield significant improvements in accuracy over simply assuming a constant value for heat capacity. The neglect of $\partial C/\partial t$ in Eq. [3] limits the value of automated heat capacity measurements.

The significance of $\partial C/\partial t$ is perhaps best illustrated by examining data from around the time of a rainfall event. On the afternoon of 24 July, 20 mm of rain fell at the bare soil site. The time courses of soil heat capacity and temperature for the 0- to 6-cm soil layer are shown in Fig. 5a. Because $\partial C/\partial t$ was significant and positive during infiltration, Eq. [3] and [4], which neglect $\partial C/\partial t$, led to large temporary underestimates of the rate of change of heat storage in the soil (Fig. 5b). During infiltration, soil temperature was decreasing while heat capacity was increasing. The change in heat storage is determined by the interplay of these counteracting processes. Equation [5] yields heat storage estimates that account for these dynamics. The other two calculation methods do not. Patterns like the ones demonstrated in Fig. 5b occurred at all three sites. The largest resulting errors in heat storage using Eq. [3] were −244 W m^{-2} at the bare soil site, −284 W m^{-2} at the soybean site, and −87 W m^{-2} at the corn site.

Neglecting $\partial C/\partial t$ also causes errors in cumulative heat storage estimates. Cumulative heat storage for 24 July at the bare soil site was −0.10 MJ m^{-2} using Eq. [5], −0.58 MJ m^{-2} using the constant heat capacity assumption, and −0.65 MJ m^{-2} using Eq. [3] (Fig. 5c). Thus Eq. [3] caused a 0.55 MJ m^{-2} underestimate of cumulative soil heat storage for the day. In a similar manner, neglecting $\partial C/\partial t$ led to small persistent overestimates of cumulative heat storage when the soil surface was
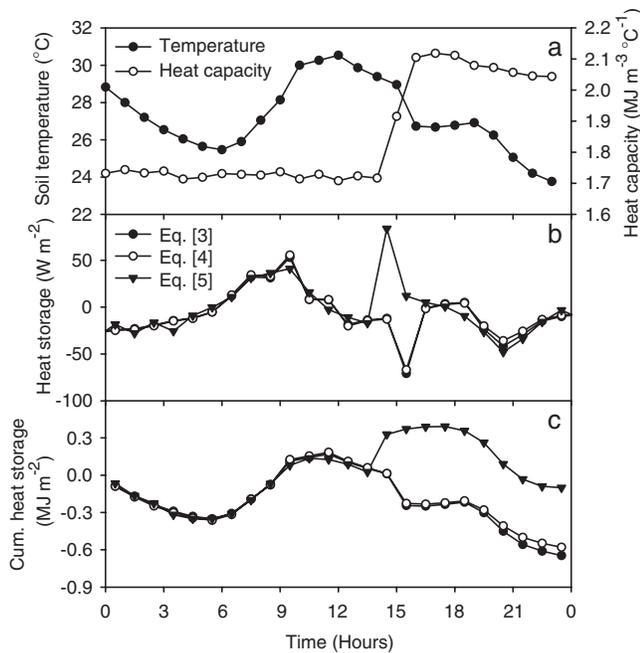
Fig. 5. Time series of (a) soil temperature and heat capacity as measured by the heat pulse sensors for the 0-to 6-cm layer at the bare soil site on July 24; (b) heat storage estimated by neglecting $\partial C/\partial t$ (Eq. [3]), by using a constant value for heat capacity (Eq. [4]), and by including $\partial C/\partial t$ (Eq. [5]); and (c) cumulative heat storage for the day using the same three approaches.

drying. For the 9-d drying period beginning on 25 July, Eq. [3] led to a 1.0 MJ m^{-2} overestimate of cumulative heat storage at the bare soil site.

Cautions Regarding Equation [5]

Two notes of caution regarding the use of Eq. [5] should be expressed. First, the measurements of heat capacity must have sufficient resolution to avoid causing unacceptably large errors in storage due to random fluctuations in the measured heat capacity between time steps. For example, consider the heat pulse sensors used at the soybean and corn sites. These sensors used Cu-constantan (Type T) thermocouples to detect the temperature rise caused by the applied heat pulse. These thermocouples produce a signal of about 40 μV °C^{-1}. The data logger resolution was 0.33 μV, so the temperature measurement resolution was about 0.0083°C. Assuming a heating power of 800 J m^{-1}, a needle spacing of 6 mm, and a soil heat capacity of 1.8 MJ m^{-3} K^{-1}, the theoretically predicted temperature rise is 1.446°C. Given the temperature measurement resolution, the reported temperature rise could be 1.454°C, in which case the heat capacity would be reported as 1.79 MJ m^{-3} K^{-1}, an error of -0.01 MJ m^{-3} K^{-1}. If the reported average heat capacity for the 0- to 6-cm layer fluctuated by -0.01 MJ m^{-3} K^{-1} during a 1-h time step in which no real change in heat capacity occurred, then the heat storage estimate would be in error by -3 W m^{-2} at a soil temperature of 20°C and -5 W m^{-2} at 30°C. For these sensors, the measured absolute change in the average heat capacity between time steps was <0.01 MJ m^{-3} K^{-1} 87% of the time, so the uncertainty in storage arising

from uncertainty in $\partial C/\partial t$ was typically <5 W m^{-2}. This uncertainty is small relative to the errors in heat storage caused by neglecting $\partial C/\partial t$, which can occasionally exceed 200 W m^{-2}.

The second caution regards the reference temperature in Eq. [5]. When heat capacity is changing with time, the heat storage value depends on the chosen reference temperature. Changes in soil heat capacity usually indicate water entering or leaving the surface soil. That mass of water carries heat with it. The quantity of heat in a given mass of water can only be specified in relation to some reference temperature. A complete energy balance would contain terms accounting for convective heat transfer by water fluxes to and from the surface (e.g., precipitation). The reference temperature dependence of these terms would balance the reference temperature dependence of heat storage in Eq. [5].

CONCLUSION

Soil heat flux is a fundamental component of the surface energy balance in terrestrial ecosystems. Accurately measuring soil heat flux requires several decisions regarding soil heat storage. Among them are: What shall the reference depth be? How will heat capacity be determined? And, how will heat storage be calculated? This study is an effort to offer some guidance on these three issues. We submit, on the basis of theoretical and empirical evidence, that when the reference depth is sufficiently deep to permit accurate heat flux measurements, heat storage is too large to neglect. We urge critical evaluation of the practice of choosing very shallow reference depths and neglecting heat storage.

On the second issue, we found that soil sampling, the ThetaProbe, and the heat pulse sensors all generally provided similar heat capacity values. Observed overestimates by the ThetaProbe in a clay soil could probably be eliminated by a soil-specific calibration. Soil sampling has inherent limitations in representing the temporal variability of heat capacity, so it does not readily facilitate the use of Eq. [5], which produces the most accurate heat storage data. Only the heat pulse sensors directly measure heat capacity, and they can also be used to monitor soil temperature. These features, along with their small size, make heat pulse sensors particularly well suited for measuring heat storage near the soil surface.

On the final question of calculating soil heat storage, we compared three different approaches: two from the literature and one new. The first and most common approach permits heat capacity to vary in time, but assumes that the time derivative of heat capacity is negligible. This approach led to occasional large underestimates of heat storage during infiltration events, with the largest such error being -284 W m^{-2}. It also gave rise to small but persistent errors during soil drying. The second and simplest approach assumes a constant value for heat capacity. This approach suffered from the same errors as the first, but the second is much easier to implement. The third approach, introduced here, includes temporal variations in heat capacity and also

includes the time derivative of heat capacity. This approach requires frequent heat capacity measurements but gives the most accurate soil heat storage data. This is especially true when soil water content is changing rapidly.

APPENDIX

The conductive heat flux, positive downward, in a homogeneous soil profile with the temperature at the surface described by a sine wave and with a constant temperature deep in the profile is given by

$$G(z,t) = A_{T}C\sqrt{\omega\alpha}\,\exp\left(-z\sqrt{\omega/2\alpha}\right)$$
$$\sin\left(\omega t + \phi + \frac{\pi}{4} - z\sqrt{\omega/2\alpha}\right) \qquad [A1]$$

where G is the heat flux, α is thermal diffusivity, and A_{T}, ω, and ϕ are the amplitude, angular frequency, and phase angle of the surface temperature wave (Horton and Wierenga, 1983). The amplitude of the heat flux wave (A) is then

$$A(z) = A_{T}C\sqrt{\omega\alpha}\,\exp\left(-z\sqrt{\omega/2\alpha}\right) \qquad [A2]$$

And the ratio of A at depth z_{r} (A_{r}) to A at the soil surface (A_{0}) is

$$\frac{A_{r}}{A_{0}} = \exp\left(-z_{r}\sqrt{\omega/2\alpha}\right) \qquad [A3]$$

To identify the time shift in heat flux with depth we take the partial derivative of Eq. [A1] with respect to time and find

$$\frac{\partial}{\partial t}G(z,t) = \omega A_{T}C\sqrt{\omega\alpha}\,\exp\left(-z\sqrt{\omega/2\alpha}\right)$$
$$\cos\left(\omega t + \phi + \frac{\pi}{4} - z\sqrt{\omega/2\alpha}\right) \qquad [A4]$$

Setting Eq. [A4] equal to 0 and solving for t, we can identify the times of the maximum and minimum values of heat flux at any depth. The time (t_{0}) of the maximum heat flux is

$$t_{0}(z) = \frac{\pi/4 - \phi - z\sqrt{\omega/2\alpha}}{\omega} \qquad [A5]$$

And the time lag between maximum heat flux at depth z_{r} and maximum heat flux at the surface is

$$t_{r} - t_{0} = \frac{z_{r}}{\sqrt{2\omega\alpha}} \qquad [A6]$$

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