NOAA Technical Memorandum NWS TDL 68

A SIMPLE SOIL HEAT FLUX CALCULATION FOR NUMERICAL MODELS

Techniques Development Laboratory
Silver Spring, Md.
May 1979

noaa NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION / National Weather Service

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A SIMPLE SOIL HEAT FLUX CALCULATION FOR NUMERICAL MODELS

Wilson A. Shaffer

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A SIMPLE SOIL HEAT FLUX CALCULATION FOR NUMERICAL MODELS

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ABSTRACT. An analytic solution of the heat equation is the basis for a scheme to compute the soil heat flux needed for a surface energy balance calculation. An initial soil temperature profile and constant thermal properties are assumed. No vertical computational levels within the soil are used or needed. The scheme is inherently accurate, since it is derived from an analytic solution and is immune from the problems of spatial truncation error and numerical instability associated with finite-difference techniques. Two simplifications of the scheme are presented that reduce computer storage requirements and the number of computations, allowing the scheme to be applied to models with a wide range of time steps.

1. INTRODUCTION

Several boundary layer and large-scale atmospheric models use an energy balance to calculate the lower boundary condition for the equation governing atmospheric temperature (Estoque, 1963; Kasahara and Washington, 1971; Long and Shaffer, 1975). Essentially, in an infinitestimally thin air-soil interface layer, the energy buildup must be zero. This implies that the sum of the net radiation, soil heat flux, sensible heat flux and latent heat flux is zero. The soil plays an important role in absorbing and storing energy during the day for release at night. Soil thermal properties determine the amount of energy that is stored and the rate at which it is either absorbed or made available.

The soil temperature is often obtained by integrating the heat equation with a finite-difference scheme. For accuracy, five or more computational levels for soil temperature are used, although Brook (1976) recently showed a transformation which reduces this number. The soil heat flux is then obtained by a finite-difference approximation to the derivative.

In all cases, the heat equation requires the specification of an initial soil temperature profile. Thermal properties for the soil are usually assumed to be constant in depth and time, either because of lack of knowledge of these properties or for convenience. Sasamori (1970) offers an interesting alternative that links soil thermal properties to soil moisture content.

The heat equation itself is parabolic and requires specification of initial conditions plus two boundary conditions. The usual lower boundary condition, applied at large depths, is that the temperature remains constant. Observations verify this--the diurnal soil temperature variation below 1 m and the yearly variation below about 10 to 15 m are negligible. At the top boundary, either the flux or the temperature may be given. With these two boundary conditions given in time, the complete soil temperature profile can be computed exactly at any time and depth. In essence, there is no need to compute temperatures within the soil. As an alternative, knowledge of the surface temperature or surface heat flux may be stored from the initial time.

2. ANALYTIC SOLUTION OF THE SOIL HEAT PROBLEM

Carslaw and Jaeger (1959) solve the heat equation,

$$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2}, \tag{1}$$

for the special case of a heat flux that varies in time, applied to one end of a semi-infinite solid with thermal diffusivity, k, and thermal conductivity, K. For the solid initially at a uniform temperature and the heat flux applied to the surface at time t,

$$F(t) = - K \left.\frac{\partial T}{\partial z}\right|_{z=0}, \tag{2}$$

Carslaw and Jaeger give the solution as a convolution integral,

$$T(z,t) = \left(\frac{k}{\pi K^2}\right)^{\frac{1}{2}} \int_0^t F(t-u) \exp\left[-\frac{z^2}{4kt}\right] u^{-\frac{1}{2}}\, du. \tag{3}$$

where u is a dummy variable of integration with dimensions of time. Generalizing (3) to the case of a non-zero initial temperature profile, $T(z,t=0) = f_0(z)$, simply adds to (3) a term we will call term 2:

$$\frac{1}{2(\pi kt)^{\frac{1}{2}}} \int_0^\infty f_0(\zeta) \left\{ \exp\left[-\frac{(z-\zeta)^2}{4kt}\right] + \exp\left[-\frac{(z+\zeta)^2}{4kt}\right] \right\} d\zeta.$$

where ζ is, again, a dummy variable.

For energy balance calculations, only the surface ($z=0$) values of temperature and soil heat flux are necessary. Eq. (3) with term 2 added yields the surface temperature as

$$T_{sfc}(t) = T(z=0,t) = \left(\frac{k}{\pi K^2}\right) \int_0^t F(t-u)u^{-\frac{1}{2}}\, du + \left[\frac{1}{\pi kt}\right]^{\frac{1}{2}} \int_0^\infty f_0(\zeta) \exp\left[\frac{-\zeta^2}{4kt}\right] d\zeta \,. \tag{4}$$

The second term on the right represents the effects of the initial temperature profile and can readily be evaluated for many analytic profiles. Table 1 gives the integral evaluated for constant, exponential, and Gaussian variations of the initial soil temperature with depth. Since the heat equation is linear, superposition of solutions holds. A linear combination of the constant, exponential, and Gaussian profiles can be used to adequately approximate most realistic initial temperature profiles.

Evaluating the first integral in (4) is more involved. We shall assume that the soil heat flux is made up of linear segments, each segment corresponding to a time increment, Δt (Fig. 1). Naturally, Δt would be a model's time step between solutions of an energy balance. We shall evaluate the integral by a trapezoidal approximation which was found to give satisfactory accuracy, while yielding easily calculated coefficients. At the time $t = n\Delta t$, $F(t-u)$ can be approximated for the increment between $i\Delta t$ and $(i+1)\Delta t$ by the linear interpolation,

$$F = F_{n-1} - \left[\frac{F_{n-i} - F_{n-i-1}}{\Delta t}\right](u - i\Delta t) \,. \tag{5}$$

The flux integral from (4) can be evaluated and simplified to

$$\alpha\left(\frac{k\Delta t}{\pi K^2}\right)^{\frac{1}{2}} \left\{F_n + \sum_{i=1}^{n-1} C_i F_{n-1} + D_n F_0\right\}, \tag{6}$$

where $\alpha = 4/3$,

$$C_i = (i+1)^{3/2} + (i-1)^{3/2} - 2i^{3/2}, \tag{7a}$$

$$D_n = (n-1)^{3/2} - n^{3/2} + \frac{3}{2} n^{1/2}. \tag{7b}$$

Table 1.--Evaluation of the soil heat term for various initial profiles.

Initial Soil Heat Profile	$\frac{1}{\sqrt{\pi kt}} \int_0^\infty f_0(\zeta) \exp\{-\zeta^2/(4kt)\} d\zeta$
$f_0 = T$ (constant)	T
$f_0 = A \exp(-Bz_{soil})$ (exponential)	Ae^{B^2kt} erfc $(B\sqrt{kt})$
$f_0 = A \exp(-Bz_{soil}^2)$ (Gaussian)	$A(1 + 4Bkt)^{-\frac{1}{2}}$

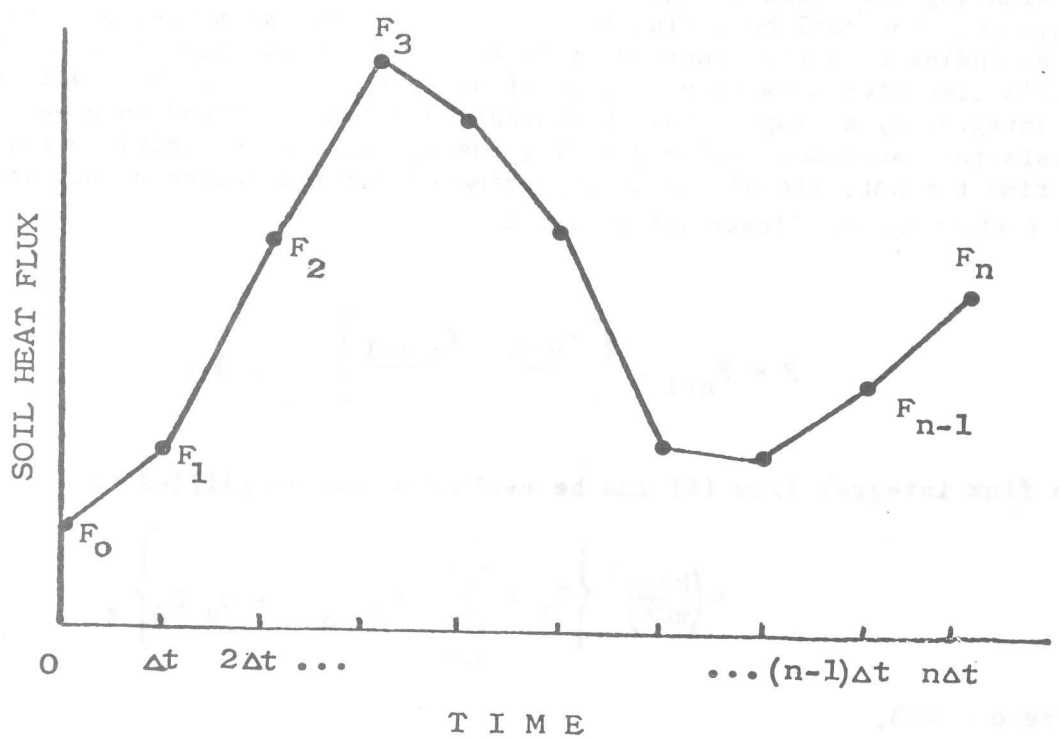

Figure 1.--Soil heat flux, assumed to be linear between each model time step, Δt. F_0 represents the soil heat flux at at time $t = 0$.

F_o is the flux at time $t = 0$ and F_i is the flux at the end of the ith step. The flux could also have been evaluated as a constant during the time increment, with its value determined by an energy balance at the end of the increment.

In this case, the coefficients are modified to

$$\alpha' = 2, \tag{8a}$$

$$C_i' = \sqrt{i+1} - \sqrt{i},$$

and

$$D_n' = 0. \tag{8b}$$

This result will be of use later when a modification to the scheme is presented.

Eq. (4) can now be inverted to give the flux as a function of the surface temperature at time step n:

$$F_n = \alpha^{-1}\left(\frac{\pi K^2}{k\Delta t}\right) T_{sfc} - \sum_{i=1}^{n-1} C_i F_{n-i} - D_n F_0 \tag{9}$$

$$+ \text{(Contribution from initial profile)}.$$

Note that the flux is a linear function of surface temperature! This form can be readily included into most energy balance solutions for surface temperature. In particular, the author uses a Newton-Raphson iterative technique in an atmospheric boundary layer model (Shaffer and Long, 1975).

3. USEFUL SIMPLIFICATIONS

The scheme presented in section 2 requires one computer storage word for each flux value at every time step. Obviously, for a three-dimensional model with a short time step, this storage demand is exorbitant. Also, the number of calculations required for each time step increases with time. Here are two modifications to the scheme that will alleviate both problems:

Method A

The integral, $\int_0^t F(t-u)^{-\frac{1}{2}} du$, from (4) may be approximated in several ways, as seen in the previous section. The resulting approximation is the sum of the product of a weighting function, C_i, and the approximate flux. The more recent fluxes are, of course, weighted more heavily than those more removed in time. The variation of C_i with i, which indicates the recentness of the fluxes, is shown in Fig. 2. Thus, at i = 1, the most recent previous flux is weighted by $C_1 = 0.823$; at i = 4, the flux 4 time steps in the past has the weight $C_4 = 0.376$; and at i = 20, the value of

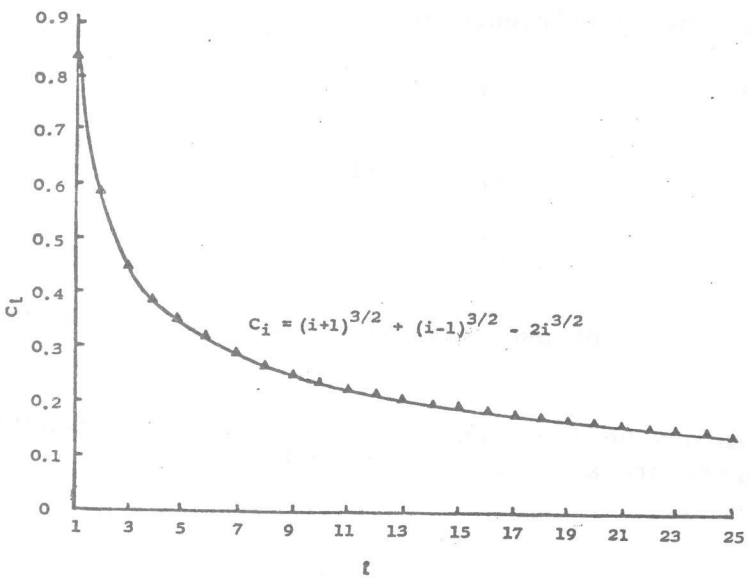

Figure 2.--Sequence used for soil flux calculations.

C_i is still 0.168. Although C_i decreases rapidly with successive recent fluxes (small values of i), its value for large i approaches zero rather slowly, so that even the "distant" past affects the current flux computation. Therefore, in general, these past fluxes should not be dropped.

Since C_i changes slowly over several steps for the distant past, several distantly past fluxes may be averaged and treated as one constant flux acting over several steps, with the appropriate weighting. In essence, the flux integral in (4) is replaced by

$$\int_0^{t_1} F(t-u)u^{-\frac{1}{2}}du + \int_{0\ t_1}^{t} \overline{F}_1\, u^{-\frac{1}{2}}du$$

where the "recent" past is defined by the time interval t_1 to t and the "distant" past by 0 to t_1. Here, $\overline{F}_1$ is the average flux between times t_1 and t = 0. As time continues, the number of unaveraged fluxes increases. Periodically averaging of the most distant remaining fluxes is desirable to reduce the number of computations. The flux integral then becomes

$$\int_0^{t_1} F(t-u)u^{-\frac{1}{2}}du + \int_{t_1}^{t_2} \overline{F}_i u^{-\frac{1}{2}}du + \ldots + \int_{t_n}^{t} \overline{F}_1 u^{-\frac{1}{2}}du$$

where $\overline{F}_i$ is the average flux in the ith averaging interval.

In practice, each time the total number of "recent" past fluxes reaches a specified number, L, an average of M of the most distant fluxes is performed. The "recent" past fluxes are treated as linear functions between time steps, as described in the previous section. The averaged fluxes act as constant fluxes for a time interval Dt = MΔt. To retain accuracy with this simplification, several of the most recent fluxes must be kept and not included in the average. Fig. 3 demonstrates how this method proceeds for values M = 6 and L = 10. With this treatment the flux calculation at time nΔt is

$$F_n = \alpha^{-1}\left(\frac{\pi K^2}{k\Delta t}\right)^{\frac{1}{2}} T_{sfc} + (\text{Contribution from initial profile})$$

$$-\left\{\sum_{i=1;\ \ell\geq 1}^{\ell} C_i F_{n-i} + D_\ell F_0 + \sum_{j=1;\ r\geq 1}^{p} C'_j \overline{F}_r\right\} \qquad (10)$$

where $p = \text{Integer}\left\{\frac{(n-1) - (L-M)}{M}\right\}$

$$\ell = (n-1) - pM,$$

and $C_i = \sqrt{A_i} - \sqrt{A_i - M}$ with $A_i = (i+1) + (p-i+1)M$.

The values of C'_j and D_ℓ are given by (8a) and (7b). Here ℓ and m are the numbers of immediately past fluxes and average fluxes, respectively, at time nΔt. When the value of ℓ reaches L, and average of the first M fluxes is made

$$\overline{F} = \frac{1}{M}\left[\frac{F_0 + F_M}{2} + \sum_{i=1}^{M-1} F_i\right]. \qquad (11)$$

Also, the value of F_o is replaced by F_M and the F_i's are renumbered, i.e., F_i replaces F_{i+M} for i=1, ..., (L-M).

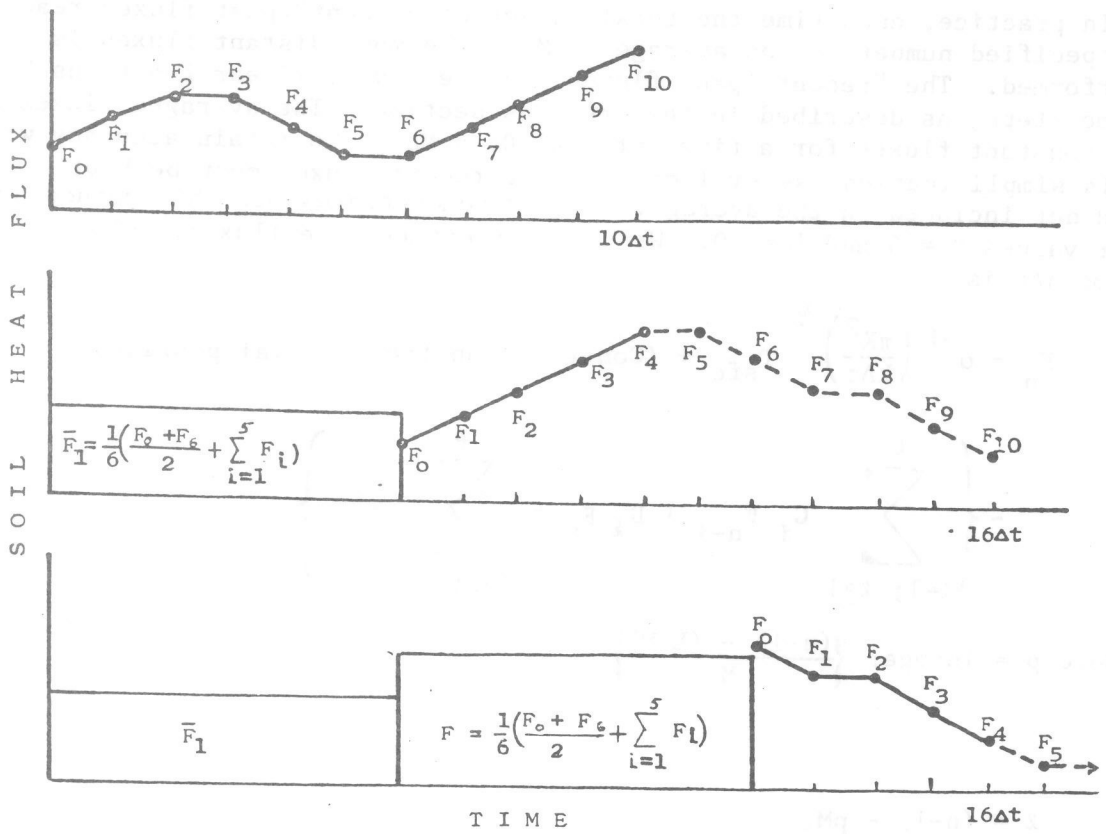

Figure 3.--Method A, with L=10 and M=6. The six most distant fluxes are averaged each time the total reaches 10. After averaging the six fluxes, the remaining fluxes are renumbered and calculations proceed.

Method B

Method A lends itself best to models which use a relatively long time step--20 minutes or longer. Now consider a model with a short time step, δt. Both the original scheme and Method A require a summation of past fluxes each time step. Method B allows this sum to be performed less frequently and does not require storing a flux each step.

Let us perform the complete flux computations every M model steps, or each $\Delta t = M\delta t$. At each increment of time $n\Delta t$, a new value of the flux will be computed and stored. Generally, at intermediate time steps, models solve an energy balance for surface temperature and thus require a value for the soil heat flux. These intermediate soil heat fluxes will be estimated values, based on a temperature extrapolated to time $(n+1)\Delta t$.

At time $n\Delta t$, the current value of the flux is stored. Also, the sum of weighted previous fluxes is performed for the new time, $(n+1)\Delta t$. At a time step $(n\Delta t + m\delta t)$ between $n\Delta t$ and $(n+1)\Delta t$, the temperature at $(n\Delta t + m\delta t)$ is obtained through an energy balance. To obtain an estimate

of the temperature at time $(n+1)\Delta t$ for the flux computation, the temperature is extrapolated from $n\Delta t$ through the value at $(n\Delta t + m\delta t)$ to $(n+1)\Delta t$. This allows an estimate of the flux at $(n+1)\Delta t$ to be computed. The estimate of the flux value at time $(n\Delta t + m\delta t)$ that is necessary in the energy balance is then the interpolated value between times $n\Delta t$ and $(n+1)\Delta t$,

$$F(n\Delta t + m\delta t) = F(n\Delta t) + \frac{F[(n+1)\Delta t] - F(n\Delta t)}{M} \; m \tag{12}$$

where

$$F((n+1)\Delta t) = \frac{3}{4}\left(\frac{\pi K^2}{k\Delta t}\right)^{\frac{1}{2}} T_{ext} + S \tag{13}$$

$$+ \text{(Contribution from initial profile)}$$

with

$$T_{ext} = T_{sfc}(n\Delta t) + M\left[\frac{T_{sfc}\,(n\Delta t + m\delta t) - T_{sfc}\,(n\Delta t)}{m}\right] \tag{14}$$

and

$$S = \sum_{i=1}^{n-1} C_i F_{n-i} + D_n F_0 . \tag{15}$$

When the time reaches $(n+1)\Delta t$, a complete flux computation is again performed. A new flux is stored and the process starts over.

Note that the summation over previous heat fluxes, S, is performed only once for the entire M time steps. Only one flux is stored for these M steps.

4. COMPARISONS

Several simple tests were run to compare the methods presented in this paper for determining the soil heat flux. In each case, a heat flux was computed for the conditions:

1) $T(t = 0,z) = 273. = \text{constant}$,

2) $T(t,z = 0) = 273. + 10. \sin\left(\frac{2\pi t}{6}\right)$, where t is in hours

3) $F(t = 0) = 0$,

4) $k = 2.3 \times 10^{-7}\ m^2/s$

and 5) $K = 1.9\ W\ m^{-1}k^{-1}$

The period of 6 hours was chosen to represent a time fluctuation which is short relative to a diurnal cycle. The 10°C amplitude yields a large temperature change over a relatively short time--a stringent test for these methods. Finally, the thermal properties were chosen as representative soil values, not values for any one specific soil type.

Various time steps (0.125, 0.25, 0.5 and 1 h) were first used to find their effect on the "exact" solution with one flux stored each step (Fig. 4). Generally, agreement is excellent after an initial transient is overcome. The transient results from shocking the soil's surface by suddenly imposing a temperature variation and cannot be resolved by using the longer time steps. Later agreement for the one-hour step is surprisingly good, considering that only six values represent the entire temperature variation for this case!

Fig. 5 compares fluxes computed by method B with M = 6, and L = 10 to those computed by the exact method with the same time step (0.125 h). Although a slight transient is introduced just after the averaging occurs, it is quickly overcome. To eliminate it, more recent fluxes may be retained. Method B is being used in an energy balance every 30 minutes within a large-scale three-dimensional boundary layer model (Long, et al., 1978). For a 24 hour (48 step) model simulation, computer storage required at each grid point is reduced from 48 to 18 flux values--10 for the most recent fluxes, seven for the averaged fluxes and one for F_0. The resulting surface temperature difference between an energy balance that uses this method and one using a flux stored each time step is generally less than 0.1°C. To use this method for short model time steps or for long model simulations, the averaging procedure can be repeated indefinitely. Several average values can later be averaged, giving a cascade of flux averages.

Method B with $\Delta t = 4\delta t$ is compared to the "exact" solution in Fig. 6. Here, $\Delta t = 0.5$ and $\delta t = 0.125$ h for Method B and $\Delta t = 0.125$ h for the exact case. Note that the fluxes computed at each Δt correspond to those from the exact solution with the same Δt. The interpolated flux obtained from this method allows an energy balance to be performed frequently, without the need of computing a sum of past fluxes each model time step.

5. SUMMARY

The soil heat calculation presented here offers an appealing alternative to integrating soil temperatures with a finite-difference approximation. First, attention is directed to the surface. No sub-soil levels are used. Unlike finite-difference approximations, the scheme avoids the question of how many computational levels are necessary for a sufficiently accurate solution. Also, no finite-difference approximation is necessary to describe the term $\frac{\partial T}{\partial z}\Big|_{z=0}$, necessary in evaluating the surface flux. Since this scheme uses no computational levels, spatial truncation errors are not involved. In addition, no stability problems have been encountered. The scheme is inherently accurate since it is based on the analytic solution of the heat equation.

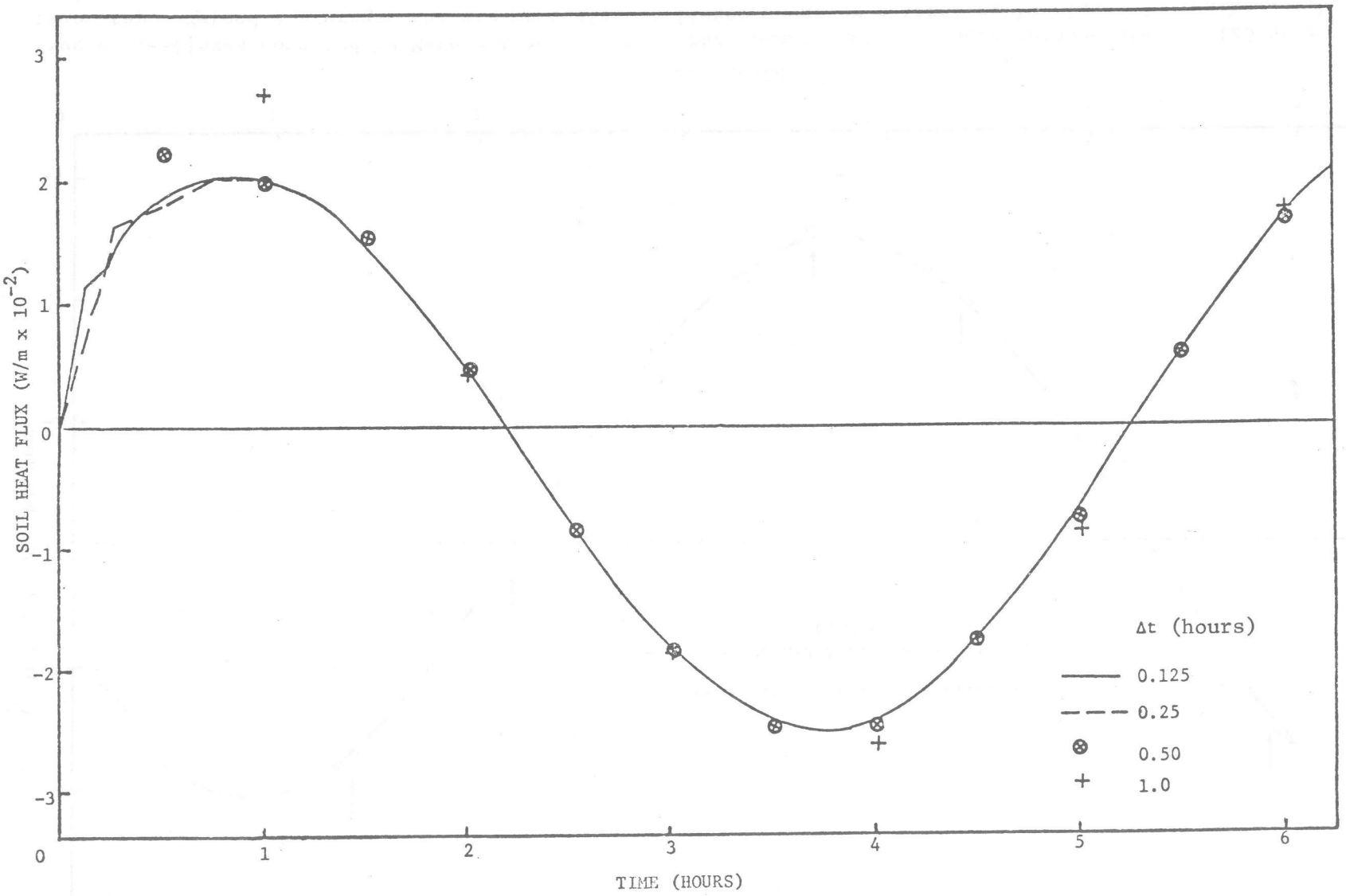

Figure 4.--Fluxes computed by the "exact" soil heat flux calculation (one flux stored each time step) for time steps of 0.125, 0.25, 0.5, and 1.0 hour. Initially, the soil is isothermal. After t=0, a sinusoidal temperature variation having an amplitude of 10°C and a period of 6 hours is imposed at the surface.

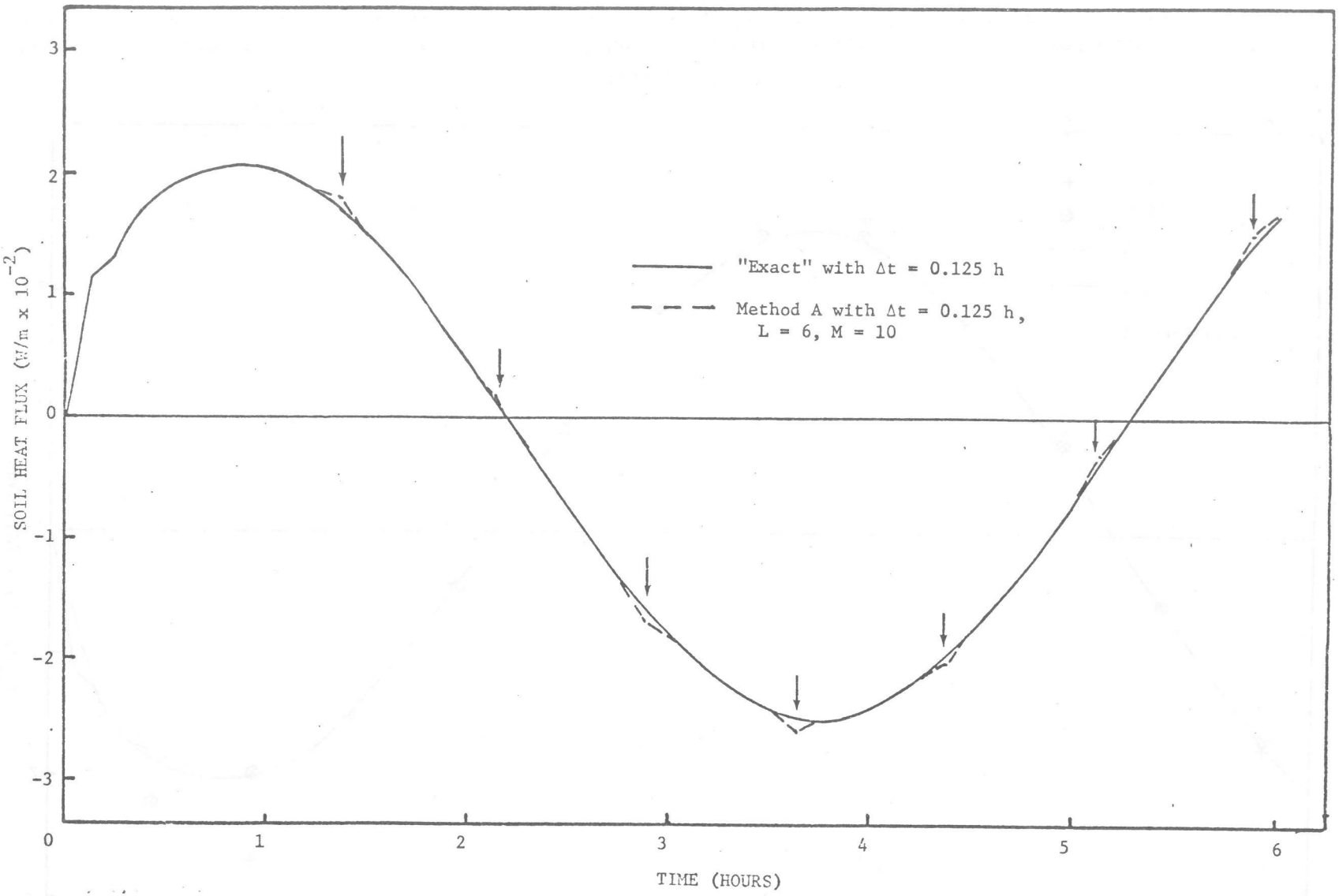

Figure 5.--Fluxes computed by Method A and those of the "exact" method. Both methods use a 0.125 hour time step. Method A averages the six most distant fluxes whenever a total of 10 fluxes is reached. The soil temperature variation is identical to that of figure 4.

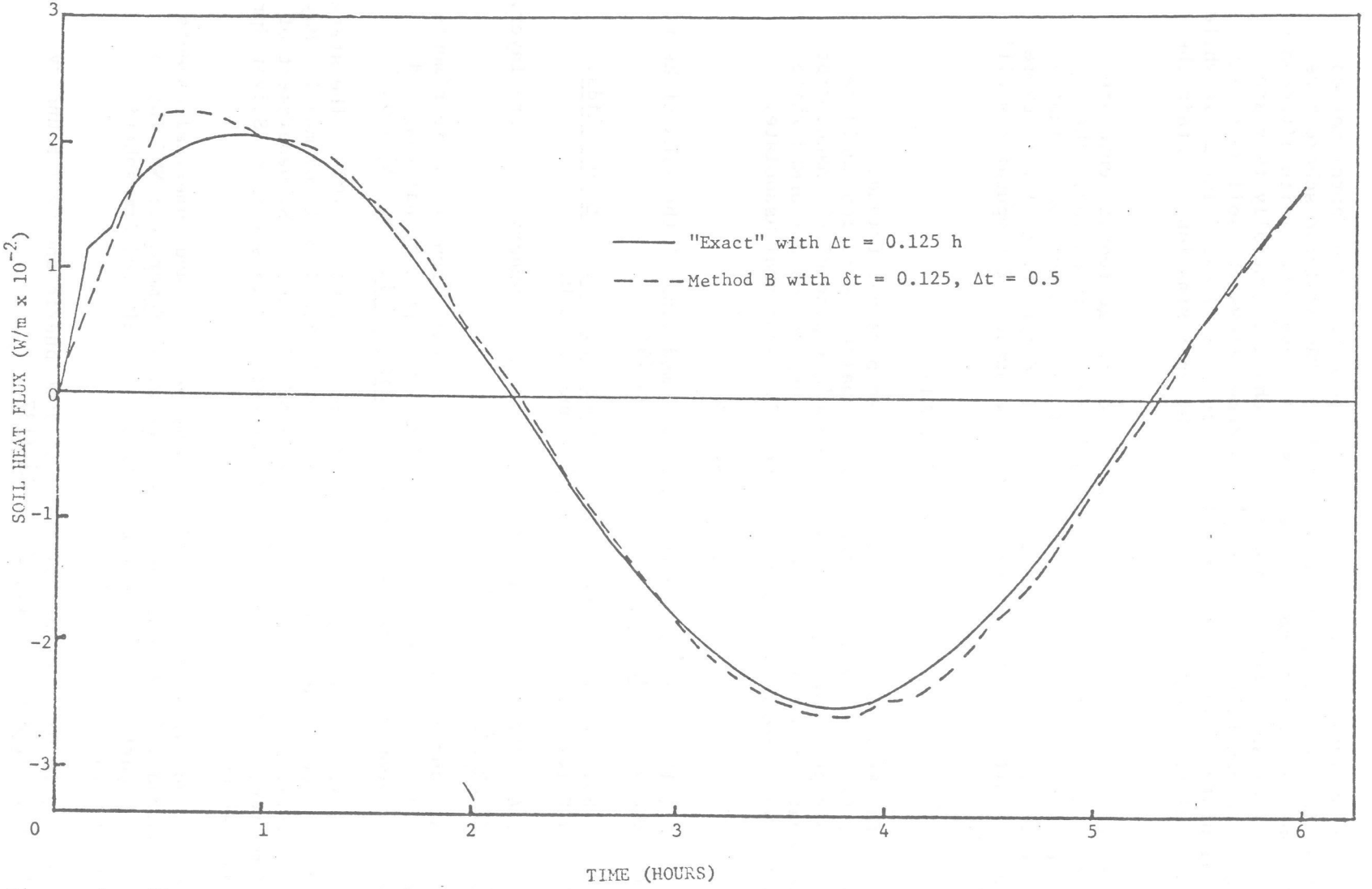

Figure 6.--Fluxes computed by Method B and those of the "exact" method. Method B requires a full flux computation only every 0.5 hour and extrapolates the temperature changes to allow flux values to be computed before the next complete interval is reached.

Both this analytic technique and the finite-difference approximation require an initial soil temperature profile. The analytic scheme here demands constant soil thermal properties. Although the finite difference approach allows soil thermal properties to change, generally they are assumed to be constants. The analytic scheme allows the soil heat flux to be calculated "exactly" through the evaluation of exact integrals while the finite-difference scheme must rely on an approximation to obtain the flux.

Two methods to reduce the computations and storage requirements are presented. These can be used individually or in combination. The coefficients of the flux terms are constant and need only be evaluated once. Generally, more storage will be required for the analytic scheme than for a finite-difference method, but the number of computations will be reduced.

6. ACKNOWLEDGMENTS

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