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Simulation of Heat Transfer in Soils[1]

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ABSTRACT

A computer model was developed to predict the temperature fluctuation in subsoil from the temperature variation at the soil surface, taking into account changes in the apparent thermal conductivity with depth below soil surface and soil temperature. The model makes use of S/360 CSMP, a recently developed simulation language for digital computers. Predicted soil temperatures were compared with soil temperatures observed at 2, 10, 15, 25, 30, and 75 cm below the surface of bare field profiles, before and after irrigation with 13.4 cm water. In wet soil observed and predicted temperatures were in close agreement. In dry soil significant differences were observed between measured and predicted soil temperatures during part of the day. The increase in apparent thermal conductivity with soil temperature had a negative effect on the magnitude of the difference between observed and predicted values in the dry soil. Agreement was found between soil heat flux density values predicted from the model and calculated with the temperature integral method. Use of a digital simulation language can save considerable programming time, and can be applied to movement of water and gases in soil profiles.

Additional Key Words for Indexing: apparent thermal conductivity, soil heat flux, digital simulation language, vapor movement.

THE TEMPERATURE variation within a soil profile is determined by the temperature variation at the soil boundaries and by the apparent thermal diffusivity of the soil. The apparent thermal diffusivity of a soil is dependent upon the soil-water content, the density, the chemical composition, and upon the temperature of the soil (5). Because in field soil profiles each of these factors changes with depths below the soil surface, the apparent thermal diffusivity is also a function of depth below the soil surface. In a previous paper (9) a numerical procedure was used to predict the temperature variation in the subsoil from the observed temperature variation at the 10-cm depth. Changes in the apparent thermal diffusivity resulting from the daily variation in soil temperature were not taken into account. Calculations made by de Vries (5) show that the apparent thermal conductivity does vary significantly with temperature. Because the temperature variation is most pronounced in surface soil, a significant error may be made in estimating the soil heat flux at the soil surface if the apparent thermal conductivity is taken constant. In the present paper, a computer model has been developed to predict the temperature of the subsoil from the temperature variation at the soil surface with values of the apparent thermal diffusivity which are dependent upon depth below soil surface and soil temperature. The computer model makes use of S/360 CSMP, a recently developed simulation language for digital computers (1, 2, 3, 7).

METHODS AND MATERIALS

Description of Computer Model

In the model the soil is divided in N layers having a thickness which increases with depth below the soil surface. A total soil depth of 125 cm was considered, divided into 50 layers with thicknesses increasing linearly from 1 mm near the soil surface to 5 cm at 125 cm. The rate of heat movement into each layer FLOWIN(I) (cal cm^{-2} min^{-1}) is a function of the temperature difference (C) between each two successive layers, the distance DX(I) (cm) between the centers of each two successive layers, and the average apparent thermal conductivity (cal cm^{-1} min^{-1} $°C^{-1}$) of the two layers KOND(I). The heat content HI(I) (cal cm^{-2}) is the product of the temperature TEMP(I), the volumetric heat capacity HCAP(I) (cal cm^{-3} $°C^{-1}$) and the thickness TX(I) (cm). The heat content of each layer at time $t + \Delta t$ is the heat content at time t plus the net rate of flow into the layer at time $t \times$ the time interval. The governing equations which describe this process of heat transfer are as follows (CSMP notation):

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HI = INTGRL(0.0, DI, 50)
TEMP(I) = HI(I)/[HCAP(I)*TX(I)]
KOND(I) = [COND(I) + COND(I-1)]/2.
FLOWIN(I)
   = [TEMP(I-1) - TEMP(I)]*KOND(I)/DX(I)
D(I) = FLOWIN(I) - FLOWIN(I+1)
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HI is a dummy variable, equivalenced to the heat content HI(I) of the layer under consideration. It represents the heat content of the layer at time $t + \Delta t$. D(I) is the net flow rate of heat into the layer. The above equations constitute the main part of the computer model. Additional equations serve to define the initial and boundary conditions, specify variables to be printed and plotted, and define the physical properties, such as water content, specific heat, bulk density, percentages of quartz and organic matter as functions of soil depth.

Values of the apparent thermal conductivity of each soil layer were calculated using the method of de Vries (4). In this method the apparent thermal conductivity, λ, is calculated from the physical properties of the soil constituents according to the weighted average:

$$\lambda = \sum_{i=0}^{n} k_i X_i \lambda_i / \sum_{i=0}^{n} k_i X_i \qquad [1]$$

where X_i is the volume fraction of each soil constituent, λ_i its conductivity, and n the number of soil constituents. The value of the weighing factor k_i depends on the shape and the orientation of the soil granules and the ratio between the conductivities of the constituents. Inasmuch as the thermal conductivity of each of the various soil constituents in equation [1] is temperature dependent (4), it is obvious that the value of the apparent thermal conductivity which is calculated for each soil layer is also temperature dependent, especially so because the influence

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TITLE SIMULATION OF SOIL HEAT TRANSFER

   STORAGE FLOWIN(51), TX(51), DX(51), X(51), HCAP(51), COND(51)
/  DIMENSION TEMP(51), HIC(51), HI(51), KOND(51), D(51)
/  EQUIVALENCE (H1, HI(1)), (HIC1, HIC(1)), (D1, D(1))
   FIXED I, NL
   PARAMETER NL = 50

INITIAL
   NOSORT
   FLOWIN(1) = 0.0
   FLOWIN(51) = 0.0
   DO 10 I = 1, NL
   FTX = I
10 TX(I) = FTX *0.1
   X(1) = 0.5* TX(1)
   DO 20 I = 2, NL
   DX(I) = (TX(I-1) + TX(I))/2.
20 X(I) = X(I-1) + DX(I)
   DO 30 I = 1, NL
   HCAP(I) = 0.5
   COND(I) = 0.0022 * 60.
   TEMP(I) = NLFGEN (TEMPT, X(I))
30 HIC(I) = TEMP(I) * HCAP(I) * TX(I)
   FUNCTION TEMPT = 0., 21.09, 5., 29.14, . . . . 125., 25.64
   FUNCTION TEMPIT = 0., 21.09, 30., 20.57, . . . . . 1440., 18.14
   H1 = INTGRL (HIC1, D1, 50)
 DYNAMIC
   NOSORT
   TEMP(1) = NLFGEN(TEMPIT, TIME)
   DO 40 I = 2, NL
   TEMP(I) = HI(I)/(HCAP(I) * TX(I))
   KOND(I) = (COND(I) + COND(I-1))/2.
40 FLOWIN(I) = (TEMP(I-1) - TEMP(I)) * KOND(I)/DX(I)
   DO 50 I = 1, NL
50 D(I) = FLOWIN(I) - FLOWIN(I+1)
   T10 = TEMP(10)
   METHOD RKS
   PRINT T10
   LABEL SOIL TEMPERATURE AT 10 CM
   PRTPLOT T10
   TIMER FINTIM = 1440., PRDEL = 30.
   END
   STOP
```

Fig. 1—Statement list of CSMP program for calculating subsurface temperature from given temperature variation at the soil surface.

of vapor movement on the conductivity is taken into account in the de Vries method. A Fortran program was written to compute the apparent thermal conductivity of each layer with equation [1], following the general procedure as outlined by de Vries (5).

In Fig. 1 the CSMP statement listing for the heat transfer problem is presented. For reasons of space the listing of the Fortran program to calculate the apparent thermal conductivity of each soil layer was omitted in Fig. 1, and a constant value given instead. For the same reasons the data on the physical properties of the soil, e.g. variation of bulk density, water content, quartz content, organic matter content with depth, were left out of the listing. The program as presented has two sections. The first section, starting with the statement INITIAL, is executed once at the beginning of the run. In the second section, starting with the statement DYNAMIC, the computations are performed repeatedly during each run under control of the selected integration routine. The Fortran deck for calculation of the thermal conductivity was inserted in the dynamic section of the model. As a result, values of the apparent thermal conductivity were updated during each iteration, or at certain time intervals, the latter depending on the rate of change of the conductivity as compared to the rate of change of the temperature of the soil. The integration method used in the program is the 4th order Runge-Kutta variable step method as specified by the statement METHOD RKS. By means of the METHOD statement, a choice may be made among seven integration methods; two of these allow the integration interval to be adjusted by the system to meet a specified error criteria. Centralized integration is used to insure that all integrator outputs are computed simultaneously at the end of a given iteration cycle. The TIMER card specifies the maximum run time (FINTIM = 1440.) and the print increment for output printing (PRDEL = 30.). The physical properties of the soil and the initial and boundary conditions were conveniently defined by tabulated values interpolated by use of non-linear function generators e.g., TEMP(1) = NLFGEN(TEMPIT, TIME). NLFGEN provides Lagrange quadratic interpolation between consecutive points in a function. More information on the various statements used in Fig. 1 can be found in the CSMP manual (7).

The above model was tested by calculating the temperature variation for uniform soil having a sinusoidal temperature variation at the surface. The results were compared with values calculated from the analytical solution (van Wijk, 1963). Because the daily temperature fluctuation is largest near the soil surface, the errors in predicting the subsurface temperature tend to be largest near the surface. By decreasing the thickness of the individual layers, the errors become smaller, but the computation time goes up. With soil layers increasing linearly from 1 mm at the surface to 5 cm at the 125-cm soil depth, it was found that the differences between values obtained from the analytical solution and the computer model could easily be made less than 0.1C at all depths, including the top layers, without requiring excessive computation time on the computer.

Measurement of Soil Temperatures

Soil temperatures were measured in three field plots of 50 sqm surface area each. Temperatures were measured at two locations at 0, 1, 2, 5, 10, 15, 20, 25, 30, 50, 75, 100, 125, and 215 cm below soil surface, and recorded at 10-min intervals during five irrigation periods in the summer of 1967. The soil-water content distribution within each plot was determined from triplicate tensiometer readings at depths of 15, 25, 50, 75, 100, and 125 cm, using the soil-water characteristic curves determined in the laboratory. Additional soil-water content measurements were made near the soil surface by gravimetric sampling at four random locations within each plot area. Samples were taken from 0 to 2.5 cm and in 5-cm depth increments from 2.5 to 17.5 cm. The quartz content, organic matter content, and specific heat were determined on composite samples taken at various depths below the soil surface. The bulk density was determined from the oven-dry weight of core samples taken from each of four pits dug just outside the plots. Further details on measurements of the temperature, the water content, and the physical properties of the soil can be found elsewhere (9).

RESULTS

Figure 2 presents soil temperature data measured 30 hours after irrigation with 13.4 cm water. The dots in Fig. 2 represent the computed soil temperatures, and the solid lines the observed soil temperatures at the various depths. The observed soil temperature at the soil surface was taken as the upper boundary for the computations. Values of the apparent thermal conductivity were calculated dependent on depth below the soil surface and temperature, using data on bulk density, percentages of quartz and organic matter as determined for this soil by Wierenga et al. (9). The calculations in Fig. 2 are based on water content values as measured at 9 a.m. There is agreement between observed and computed soil temperatures. Near the end of the day the observed soil temperatures are generally higher than the predicted soil temperatures. This may have been caused by the drying of the soil surface during the day, since in the calculations a constant soil-water content was assumed. Soil temperature data for the same location before irrigation are presented in Fig. 3. The differences between ob-

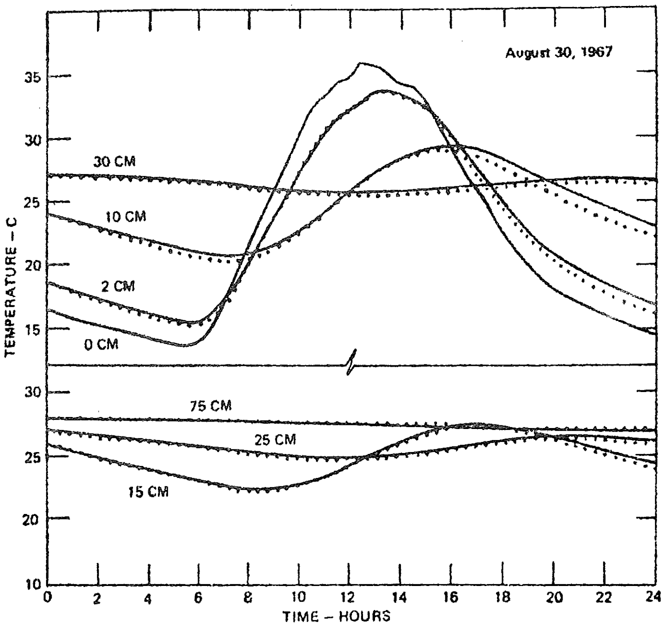

Fig. 2—Observed and calculated soil-temperature variation in wet soil at 0, 2, 10, 15, 25, 30, and 75 cm. The solid lines are the observed soil temperatures. The dots represent the computed soil temperatures.

served and computed soil temperatures are now considerably larger than for wet soil. It appears that the values of the apparent thermal conductivity calculated with the de Vries method are too high.

In Table 1 values of the apparent thermal conductivity used to calculate the temperature variation of the soil before irrigation (Fig. 3) are presented at 6 hour time intervals for depths of 1, 2, 5, 10, and 25 cm. It is apparent that the de Vries method results in appreciable variation in the thermal conductivity with temperature or time of day. This is especially the case for intermediate water contents. Below 25 cm the variation in thermal conductivity with time of day is negligible because of the higher water content at those depths and the small temperature fluctuation.

Table 2 shows for the nonirrigated soil the differences between observed and computed soil temperatures. The computed soil temperatures were obtained with temperature dependent (TD) conductivity values, and with temperature independent conductivity values (NTD) using an average soil temperature of 30C. The data show that the difference between observed and computed soil temperature is greater for soil temperatures computed with temperature dependent values of the apparent thermal conductivity.

The soil heat flux density is calculated in the computer

Table 1—Variation of apparent thermal conductivity (mcal cm^{-1} sec^{-1} $°C^{-1}$) with the time of the day, computed at five depths below the soil surface

Time-hours	Soil depth, cm				
	1	2	5	10	25
0	0.78	1.06	1.86	2.58	3.22
6	0.76	1.02	1.77	2.49	3.21
12	0.95	1.29	2.05	2.62	3.19
18	0.82	1.15	2.00	2.68	3.22
24	0.76	1.04	1.81	2.54	3.22
Water content (cm^3/cm^3)	0.02	0.04	0.10	0.21	0.32

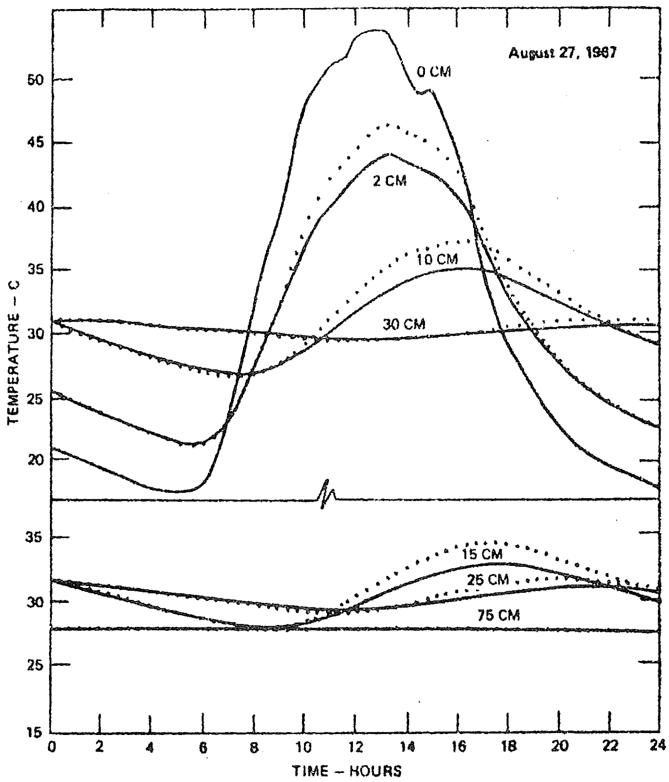

Fig. 3—Observed and calculated soil-temperature variation in dry soil at 0, 2, 10, 25, 30, and 75 cm. The solid lines are the observed soil temperatures. The dots represent the computed soil temperatures.

model as the product of the temperature gradient between layers 1 and 2 and the average apparent thermal conductivity of the two layers. Because the thickness of the first layer is only 1 mm, the amount of heat stored in this layer is very small and can be neglected for the purpose of computing the total soil heat flux density. The soil heat flux densities for the temperature data of Fig. 2 and 3 are presented in Fig. 4. The soil heat flux density computed with the temperature integral method is also given. In this method the soil heat flux for a given time interval is the sum of products of the volumetric heat capacity times the temperature change for each soil layer. The volumetric heat capacity was determined from the water content and the specific heat of the soil profiles. Because the soil temperature profile was measured every 10 min at 13 depths below the surface, this method should yield an accurate estimate of

Table 2—Difference between observed and computed soil temperatures at various times of the day at 2, 10, and 30 cm below soil surface. The computed values were obtained with values of the apparent thermal conductivity which were either dependent on soil temperature (TD) or not dependent on soil temperature (NTD)

	Soil depth, cm	Time, hours				
		0	6	12	18	24
Obs.-comp. (TD)	2	0	0	-2.3	-0.8	-0.1
Obs.-comp. (NTD)	2	0	-0.1	-1.9	-0.6	0.1
Obs.-comp. (TD)	10	0	0.3	-1.5	-1.5	-0.2
Obs.-comp. (NTD)	10	0	0.4	-1.0	-1.1	0.1
Obs.-comp. (TD)	30	0	0.2	0.2	-0.4	-0.3
Obs.-comp. (NTD)	30	0	0.2	0.2	-0.2	-0.2

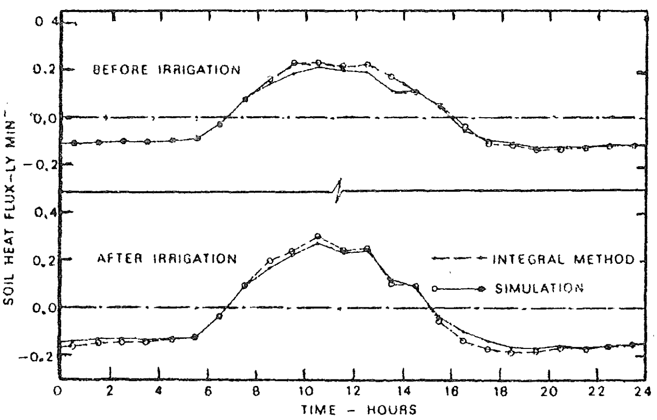

Fig. 4—Soil heat flux density data computed by the integral method and by the simulation method for dry and wet soil conditions.

the soil heat flux density. Figure 4 shows that soil heat flux data obtained from the two methods are in close agreement.

DISCUSSION

The data show that with the knowledge of the physical properties of the soil a good estimate can be made of the variation in subsoil temperature from the temperature fluctuation at the soil surface or at some level below. In de Vries' method for calculating the thermal conductivity, as used in the present model, heat conduction by vapor transfer is accounted for by assuming that the vapor flux due to temperature differences is to a good degree of approximation proportional to the temperature gradient across a gas-filled pore (de Vries, 5). The value of the apparent conductivity that is calculated is therefore partly due to normal heat conduction and partly due to vapor movement. However, changes in the thermal conductivity of water and of the solid phase of the soil with temperature are relatively small. Thus vapor movement, assumed to be proportional to the temperature gradient, is the probable mechanism that causes the daily fluctuation in the apparent thermal conductivity as presented in Table 1. Comparison of the observed and computed soil temperatures on August 27 shows that the differences between observed and computed values are initially small, increase around 10 a.m., and decrease again after the soil temperature reaches its maximum. This behavior was observed in all three plots of the experiment. The differences between observed and computed soil temperatures in the nonirrigated surface soil become less if the apparent thermal conductivity is either constant (Table 2) or becomes smaller with increasing soil temperature. Inasmuch as the differences between observed and computed soil temperatures are small for wet soil, this indicates that for soil of intermediate water content heat transfer processes other than those used in the model are of some importance, e.g. the thermal effects of vapor movement by temperature gradients. The net result of these effects is a decrease in the apparent thermal conductivity with temperature.

From the soil heat flux data in Fig. 4 it is obvious that with the computer model a good estimate can be made of the hourly values of the soil heat flux density. The data compare favorably with those of Staley and Gerhardt (8) and Gerhardt (6) who found at O'Neill, Nebraska that the heat flux density values measured with the various methods differed by more than 100%, both under wet and dry soil-water conditions.

It was found in developing the model described in this paper that S/360 CSMP is a convenient language for simulating heat transfer in soils. Although many of the features used in this model can be programmed in Fortran, considerable programming time may be saved by using a digital simulation language such as CSMP. The savings made on programming time will easily offset the increased cost of computation time. It is felt that digital simulation languages are equally useful in describing water flow in soil under both saturated and unsaturated conditions and may be used also for estimating the evaporation and evapotranspiration from bare and cropped surfaces from climatological data. In general, the use of continuous system simulation languages will allow more complex systems to be handled with the same or less programming effort.

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