Contributions to Methodology and Statistics
A. Ferligoj and A. Kramberger (Editors)
Metodološki zvezki, 10, Ljubljana: FDV 1995

Dynamic Model MEBIT for Simulation of Soil Physical Processes

Damjana Kastelec[1]

Abstract

Dynamic model MEBIT was constructed to predict the soil temperature and the soil moisture depending on calender time and on soil depth. Model is based on physical laws of heat conduction, water vapour diffusion and water mass flow in vertical direction as well as upon some empirical investigation on thermal and hydraulic properties of soil.

A system of two nonlinear differential equations is solved using Runge-Kutta fourth order numerical method with variable computing time step. The system of two nonlinear differential equations is simplified by the assumption that thermal and hydraulic properties in horizontal direction are constant. The boundary conditions in vertical direction are set with the energy balance equation at the soil surface and with the constant soil temperature and non-existant water flow at the bottom soil layer.

For the purpose of illustration the model was applied to the data from agrometeorologic weather observation station in Bilje, during the spring season.

1 Introduction

Several investigations in soil physics, agrometeorology, pedology and biology indicate that almost all biological, chemical and physical processes in a particular soil type are predominatly influenced by the soil temperature and by the soil moisture. The soil temperature and the soil moisture depend on weather conditions above the soil surface as well as on physical and chemical properties of soil, such as heat conduction, heat capacity, hydraulic conductivity, texture and structure.

Some physical laws explain the variations of the soil temperature and the soil moisture. Several empirical, semi-empirical and theoretical models were made to predict changes of the soil temperature and the soil moisture during infiltration, redistribution or drainage of water in different types of soil, under different weather conditions. The most commonly used models are based on the physical theory of heat conduction, vapour diffusion and water mass flow in the soil (Philip and de Vries, 1957; 1958) as well as on some empirical investigations of soil thermal

[1]Office for Meteorology and Hydrology of Slovenia, Vojkova 1b, 61000 Ljubljana, Slovenia

and hydraulic properties (de Vries, 1963; McInnes, 1981; Milly and Eagleson, 1980; Genuchten, 1980; Campbell, 1985; Saxton et al., 1986). This physical theory can be expressed as a system of two differential equations whith no analytical solution. A numerical method is used to find a stable solution for the chosen boundary and initial conditions (Jury and Miller, 1974; Babel in Hillel, 1976; Milly and Eagleson, 1980; Firdaouss in Caussade, 1981; Horton and Wierenga, 1984; Campbell, 1985; ten Berge, 1990; Benjamin, 1990).

In this paper we present a new model MEBIT (Masna in Energijska BIlanca Tal), (Virant, 1993), which is constructed for agrometeorological purposes. Like the models mentioned above, it is based on physical laws and empirical investigations. The aim of our work was to construct a model which would give the best possible results, applying the commonly used data for describing weather conditions and soil type. In our circumstances the most suitable way of achieving that was to use hourly values of meteorological variables from automatic meteorological observation stations and soil texture and organic matter content as input data. The soil layer was considered to contain inhomogeneities of thermal and hydraulic properties of soil in a vertical direction.

2 Physical theory

Both the soil temperature and the soil moisture have characteristic fluctuations throughout the years. These are dependant upon weather conditions above the soil surface as well as on the thermal and hydraulic properties of the soil. The soil thermal properties - thermal conductivity and heat capacity depend also on the soil moisture. On the other hand, soil hydraulic properties are also dependent upon soil temperature. There is an interdependance between water mass and heat flow in the soil, which must be taken into account when modelling soil physical processes.

In some cases horizontal homogeneity of thermal and hydraulic properties in the soil can be assumed. With this assumption the problem is reduced to soil water mass and heat flow in vertical direction only. The physical theory can be expressed in a mathematical form as a system of two nonlinear differential equations as follows in Eq. (1) and (2). The equation for time and space variations of the soil temperature is

$$\frac{\partial(C(\theta)T)}{\partial t} = \frac{\partial}{\partial z}(\lambda(\theta)\frac{\partial T}{\partial z}) + L\frac{\partial}{\partial z}(D_e(\theta,T)\frac{\partial \varrho_v(\theta,T)}{\partial z}). \tag{1}$$

θ - volumetric water content (m^3/m^3),
$C(\theta)$ - volume heat capacity (J/m^3K) (de Vries, 1963),
T - soil temperature (K),
$\lambda(\theta)$ - heat conductivity (W/mK), (de Vries, 1963; McInnes, 1985),
$D_e(\theta,T)$ - effective soil water vapor diffusivity (m^2/s),
L - water latent heat (J/kg),
ϱ_v - water vapour density (kg/m^3),
z - space dimension in vertical direction (m), positive downward,
t - time variable (s).

The first term of the right side of the equation represents the soil temperature variations due to heat conduction in the soil. The second term the soil temperature variations due to heat flow with water vapour diffusion.

The equation for the time and space variations of the soil water content, if the soil moisture is expressed by volumetric water content θ, is

$$\varrho_l \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}(K(\theta)\frac{\partial \psi(\theta)}{\partial z}) - \varrho_l g \frac{\partial}{\partial z} K(\theta), \quad (2)$$

g - gravitation acceleration (m/s^2),
$K(\theta)$ - soil hydraulic conductivity $(kg/(msPa))$, (Saxton et al., 1986; Campbell, 1985; Mualem, 1976),
$\psi(\theta)$ - soil water potential (Pa),
ϱ_l - liquid water density (kg/m^3).

Other quantities are denoted as in Eq. (1). The relation between soil water potential and volumetric water content is specific for each soil type and is usually described by means of empirical determined soil desorption curve $(\partial\psi/\partial\theta)$, (Saxton et al., 1986; Campbell, 1985).

Equation (2) can be replaced by equation (3) when there is no water flow and there is only vapour diffusion in the soil.

$$\varrho_l \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}(D_e(\theta, T)\frac{\partial \varrho_v(\theta, T)}{\partial z}). \quad (3)$$

D_e - effective soil water vapour diffusivity (m^2/s), (Philip and de Vries, 1957; Cary, 1963).

The first term on the right of Eq. (2) represents the soil water content variations caused by capillary forces, the second term represents the soil water content variations caused by gravity force. The water vapour diffusion is caused by soil air humidity gradient (Eq. 3).

In MEBIT, the soil thermal and hydraulic properties used in Eq. 1, 2 and 3 ($\lambda(\theta)$, $C(\theta)$, $K(\theta, T)$), and the soil desorption curve $(\partial\psi/\partial\theta)$ are determined by the same empirical and semi empirical relations as in de Vries (1963), Campbell (1985), McInnes (1985), and Saxton et al. (1986).

Formulating MEBIT the following additional basic restrictions were imposed:
- no vegetation cover on the soil surface,
- no sinks or sources of heat and water mass in the soil,
- no runoff on the soil surface,
- no effect of ground water.

3 Method for numerical solution

3.1 Space integration

In MEBIT, the whole soil layer (z_b on Figure 1), is divided into sublayers with different texture and organic matter content and consequently with different thermal

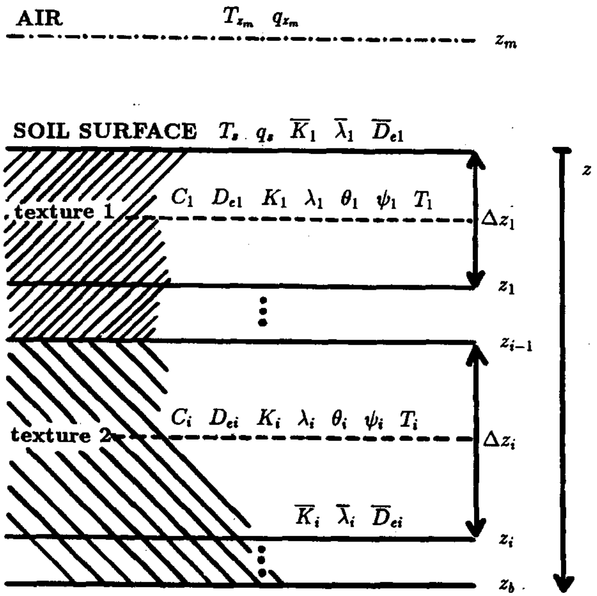

Figure 1: The arrangement of the variables in the model space used by space integration in MEBIT. The variables are denoted as in the text.

and hydraulic properties. The number and thickness of sublayers depend on soil type. At the boundaries between the soil sublayers there is a vertical discontinuity of the soil volumetric water content.That discontinuity causes difficulties in the mathematical formulation of boundary conditions. Therefore it is more convenient to use the soil water potential with no discontinuity as the prognostic variable.

Because of numerical integration in MEBIT, the whole soil layer (z_b) is divided into a chosen number of computational sublayers (Δz_i, $i = 1...b$ on Figure 1). The thickness of computational sub layers is determined for each simulation separately, depending on the soil type and weather conditions, with respect to the stability of the numerical method. Near the soil surface the thickness of the computational sublayers is small and increases with depth. This is due to great soil temperature gradient and great soil moisture gradient, that occur near the soil surface.

However, if the whole soil layer (z_b) has sublayers with different physical properties, the computational sublayers are determined in a way that some of the boundaries between the computational sublayers coincide with the boundaries of sublayers with different physical properties (see Figure 1).

For the space integration, Eq. 1, 2, and 3 are written in the following numerical form (Eq. 4, 5, 6):

$$\frac{\partial(C_i(\theta)T_i)}{\partial t} = \frac{\overline{\lambda}_{i+1}\frac{T_{i+1}-T_i}{0.5(\Delta z_i+\Delta z_{i+1})} + L\overline{D}_{e_{i+1}}\frac{\varrho_{v_{i+1}}-\varrho_{v_i}}{0.5(\Delta z_i+\Delta z_{i+1})}}{\Delta z_i} - \frac{\overline{\lambda}_i\frac{T_i-T_{i-1}}{0.5(\Delta z_{i-1}+\Delta z_i)} - L\overline{D}_{e_i}\frac{\varrho_{v_i}-\varrho_{v_{i-1}}}{0.5(\Delta z_{i-1}+\Delta z_i)}}{\Delta z_i} \quad (4)$$

$$\varrho_l\frac{\partial\theta}{\partial t} = \frac{-\overline{K}_{i+1}\frac{\psi_i-\psi_{i+1}}{0.5((\Delta z_i+\Delta z_{i+1})} + \overline{K}_{i+1}\varrho_l g + \overline{K}_i\frac{\psi_{i-1}-\psi_i}{0.5((\Delta z_{i-1}+\Delta z_i)} - \overline{K}_i\varrho_l g}{\Delta z_i} \quad (5)$$

$$\varrho_l\frac{\partial\theta}{\partial t} = \frac{\overline{D}_{e_{i+1}}\frac{\varrho_{v_{i+1}}-\varrho_{v_i}}{0.5(\Delta z_i+\Delta z_{i+1})} - \overline{D}_{e_i}\frac{\varrho_{v_i}-\varrho_{v_{i-1}}}{0.5(\Delta z_{i-1}+\Delta z_i)})}{\Delta z_i} \quad (6)$$

where index i represents space coordinates (Figure 1), $i = 1...b$.

Figure 1 represents the model space. Dashed lines represent the middle of sublayers. There, the prognostic variables (θ_i, ψ_i, T_i), their time derivatives and the soil thermal and hydraulic properties $(C_i, \lambda_i, K_i, D_{e_i})$ are computed. The solid lines are boundaries of the computational sublayers, where energy and mass fluxes and averages of thermal and hydraulic properties $(\overline{\lambda}_i, \overline{K}_i, \overline{D}_{e_i})$ are computed. The past investigations (Haverkamp and Vauclin, 1979) of calculating the thermal and hydraulic properties of soil showed that it is convenient to use the weighted average for the heat conductivity ($\overline{\lambda}_i$, Eq. 7):

$$\overline{\lambda}_i = \frac{\lambda_{i-1}\Delta z_{i-1} + \lambda_i\Delta z_i}{\Delta z_{i-1} + \Delta z_i} \quad (7)$$

and geometric average for the hydraulic conductivity ($\overline{K}_i$, Eq. 8) and effective water vapour diffusivity ($\overline{D}_{e_i}$, Eq. 9):

$$\overline{K}_i = \sqrt{K_{i-1}K_i} \quad (8)$$

$$\overline{D}_{e_i} = \sqrt{D_{e_{i-1}}D_{e_i}} \quad (9)$$

3.2 Integration over time

The system of Equations (4) and (5) or (4) and (6) is solved using variable computational time step Runge-Kutta fourth order numerical method which gives the following time integration scheme (Berge, 1990; Bohte, 1985):

$$\begin{aligned} A^{p_1} &= A^n + \Delta t f(A^n)/2 \\ A^{p_2} &= A^{p_1} + \Delta t f(A^{p_1})/2 \\ A^{p_3} &= A^{p_2} + \Delta t f(A^{p_2}) \\ A^{n+1} &= A^n + \Delta t(f(A^n) + 2f(A^{p_1} + 2f(A^{p_2}) + f(A^{p_3}))/6 \end{aligned} \quad (10)$$

A is one of the prognostic variables (T, θ), n is the stage at the end of the previous step of integration, $n+1$ is stage of the instantaneous step of integration;

p_1, p_2, p_3 denote the transient stages of integration, f is numerical form of one of the prognostic equations (Eq. 4, 5, 6). The time step (Δt) is determined by the CLF criterion, which is commonly used in numerical methods in meteorology:

$$\Delta t = \alpha \; min_{i=1...b}(C_i \Delta z_i^2 / \lambda_i). \tag{11}$$

In order to obtain numerical stability, C_i, λ_i and Δz_i are volumetric heat capacity, heat conductivity and thickness of the $i-th$ computational sublayer; α is the factor which is used to control convergence, and in MEBIT it has the value 0.5. The operator min finds minimum value of the function in brackets over all the computational layers.

3.3 Boundary and initial conditions

In the case of MEBIT the boundary conditions for soil temperature and soil moisture at the soil surface are determined by the energy and mass balance equations. The energy balance equation is

$$R_s + R_{la} + R_{ls} + H + LE + G = 0 \tag{12}$$

R_s - solar global radiation (W/m^2),
R_{la} - long wave radiation of atmosphere (W/m^2),
R_{ls} - long wave radiation of soil surface (W/m^2),
H - sensible heat (W/m^2),
LE - and latent heat (W/m^2),
G - conduction of heat in the soil (W/m^2).

The energy fluxes of R_{ls}, H and G depend on soil surface temperature (T_s) and Equation (4) can be written as the function of (T_s):

$$R_s + R_{la} - \epsilon_s \sigma T_s^4 + \varrho c_p \frac{T_{z_m} - T_s}{r_{ah}} - \overline{\lambda}_1 \frac{T_{z_m} - T_s}{z_m} = 0 \tag{13}$$

ϵ_s - soil surface emissivity depending on soil moisture,
σ - Stefan-Boltzman constant ($WK^{-4}m^{-2}$),
ϱ - air density (kg/m^3),
c_p - air specific heat capacity (J/kgK),
T_{z_m} - air temperature at z_m high (K),
r_{ah} - aerodynamic sensible heat resistance, dependant upon the stability of the atmosphere (s/m), (Businger, 1975),
$\overline{\lambda}_1$ - average soil heat conductivity at the soil surface (W/mK).

The boundary condition for soil temperature at the soil surface (T_s) is determined by iterative solution of Equation (4). At the beginning of the iteration T_s is equal T_1 from the last time integration step.

The boundary condition for the soil volumetric water content at the soil surface is determined by the equation of water mass balance in the first computational layer:

$$P + E + F_k + F_g = 0 \tag{14}$$

P - precipitation intensity $(kg/(m^2s))$,
E - evaporation at the soil surface $(kg/(m^2s))$,
F_k - water mass flow in the soil due to capillary forces $(kg/(m^2s))$,
F_g - water mass flow in the soil due to gravity force $(kg/(m^2s))$.

In the second boundary condition the soil temperature (T_b) at the bottom of the soil layer (z_b) is kept constant during the simulation time and water or vapour mass flow through the bottom boundary level (z_b) is set to 0:

$$z = z_b, \quad T_b = const., \quad (\frac{\partial \theta}{\partial z})_{z_b} = (\frac{\partial \varrho_v}{\partial z})_{z_b} = 0 \tag{15}$$

At the beginning of each simulation, the initial conditions are determined by the soil temperature and volumetric water content in the middle of each computational layer.

3.4 Input data

MEBIT uses input data that describe weather conditions and soil type. The input data representing weather conditions are hourly values of air temperature, relative humidity, pressure, wind velocity, global radiation and precipitation. Usually we can get data in an appropriate form from an automatic meteorological observation station. The input data describing soil type are texture, organic matter content and thickness of soil layer.

4 Description of the model

For computer application, MEBIT is written in Pascal. It can be run on PC (386 or 486) or on work station (HP Appolo series 700). The computer program consists of four main parts. The first part includes initialization procedures, the second part procedures for soil heat flow simulation. In the third part, the procedures for soil water mass flow are included and in the fourth time integration and output file construction take place. The output files include predicted hourly values of the soil temperature, volumetric water content, soil water potential, soil heat and water mass flow for the chosen computational layers. These files are suitable for a graphic representation of the results in Quattro Pro or in other graphical programs.

5 Presentation of some results

The application of the model was done for eutric cambic soils at the meteorological observation station in Bilje in the south-west of Slovenia. The whole soil layer is 0.7 m deep and it consists of three soil sublayers with different physical properties. This type of soil is very common in Slovenia and is suitable for agricultural work. The depth of the bottom boundary of the whole soil layer should be determined with respect to the assumption of no ground water influence in the model. The

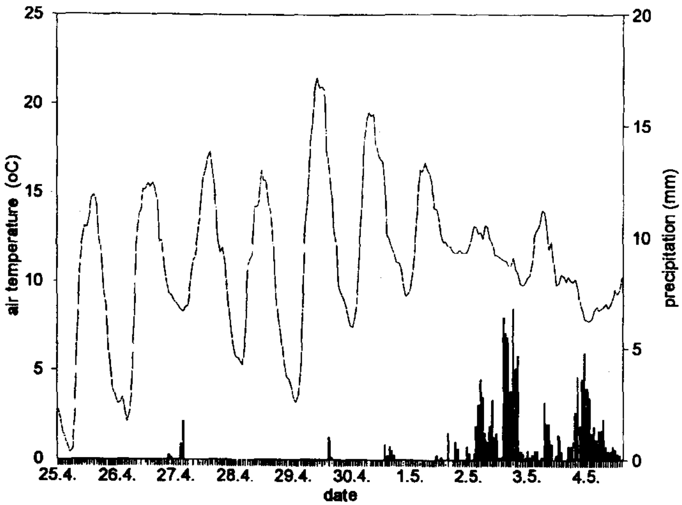

Figure 2: Hourly values of air temperature and precipitation in Bilje, 25th April to 4th May, 1991.

thickness of the computational sublayers was determined due to the stability of the numerical solution with heuristic approach. It was found that the thickness of the first computational sublayer under the soil surface has the greatest influence on the solution stability.

The comparison between predicted and measured values of soil temperature showed that MEBIT gave good results in the five day simulations. The CPU time in five day simulation is about 5 minutes on HP Appolo 730 work station.

The simulation was performed during the period 25^{th} April to 4^{th} May 1991 (see Figure 2). Weather conditions were representative for this time of the year in Bilje.

For the chosen conditions, MEBIT gives stable results if the thickness of the first computational layer is about 0.01 m and the time step is about 600 s. Two five day simulations were made. Figure 3 and 4 represent model output hourly values for soil temperature and soil moisture, in six different soil depths.

6 Conclusion

MEBIT was made to simulate soil temperature and soil moisture variations in a vertical direction in different soil types and under different weather conditions. The physical properties of the soil such as heat conductivity, heat capacity, hydraulic

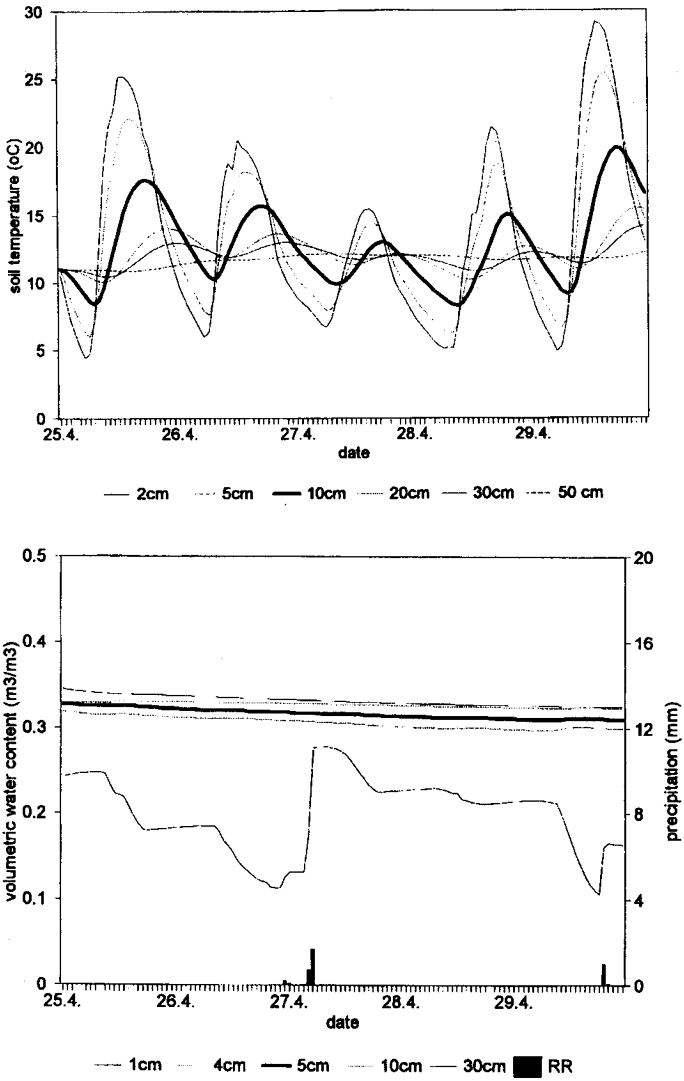

Figure 3: Hourly values of the soil temperature (top) and the soil volumetric water content (bottom) in different soil depths, computed with MEBIT for the period from 25^{th} to 29^{th} April 1991, in Bilje.

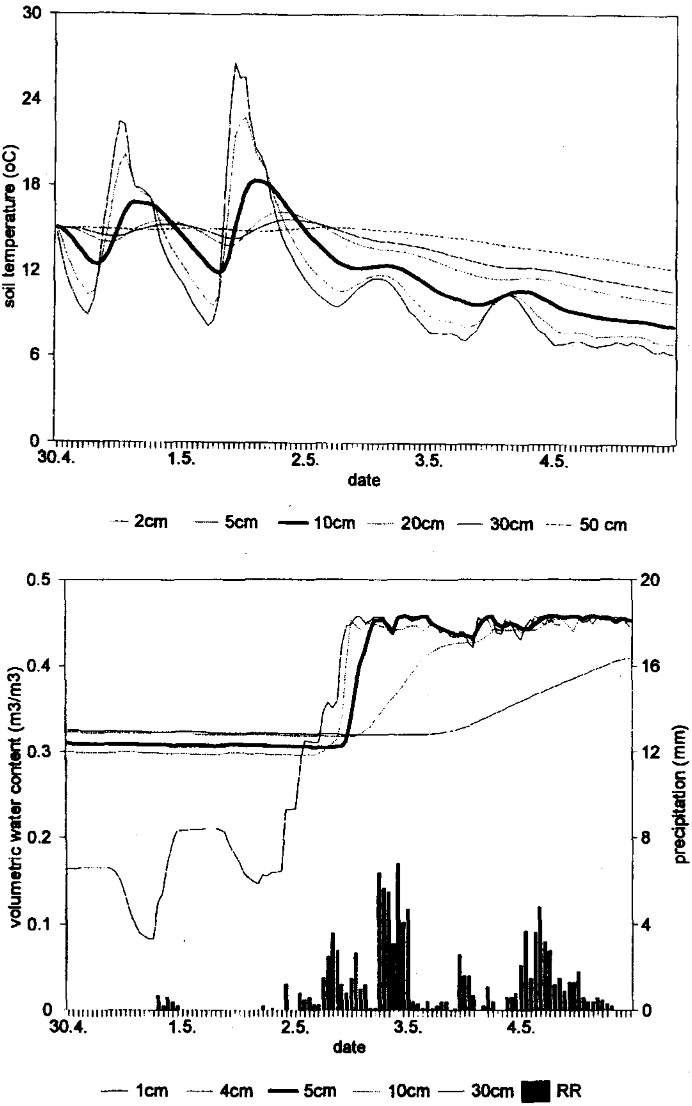

Figure 4: Hourly values of the soil temperature (top) and the soil volumetric water content (bottom) in different soil depths, computed with MEBIT for the time period from 30^{th} April to 4^{th} May 1991, in Bilje.

conductivity, and desorption curve, are determined by empirical or semiempirical relations (de Vries, 1963; Saxton et al., 1986; Campbell, 1985). They depend on soil texture, organic matter content and water content.

To solve the system of two nonlinear differential equations the variable computation time step Runge-Kutta fourth order numerical method was found as the most suitable method to get a stable solution. The stability of the space integration depends, first of all, on the thickness of the first computational layer under the soil surface. In MEBIT, this thickness is determined heuristicaly and it depends on soil type and weather conditions.

In further work the model could be adjusted for other agrometeorologic weather stations.

References

[1] Bavel, C.H.M. van, and Hillel, D.I. (1976): Calculating Potential and Actual Evaporation from a bare Soil Surface by Simulation of Concurrent flow of Water and Heat. *Agricultural Meteorology*, **17**, 453 - 476.

[2] Benjamin, J.G., Ghaffarzadeh, M.R., and Cruse, M.R. (1990): Coupled Water and Heat Transport in Ridges Soils. *Soil Sci. Soc. Am. J.*, **54**, 963 - 969.

[3] Berge, H.F.M. ten, and Bolt, G.H. (1988): Coupling between Liquid Flow and Heat Flow in Porous Media: A Connection between Two Classical Approaches. *Transport in Porous media*, **3**, 35 - 49.

[4] Berge, H.F.M. ten (1990): *Heat and Water transfer in Bare Topsoil and the Lower Atmosphere.* Wageningen: Pudoc.

[5] Biotehniška fakulteta (1984): *Študija evapotranspiracije za potrebe namakanja kmetijskih zemljišč v Vipavski dolini.* Ljubljana: Biotehniška fakulteta Univerze v Ljubljani.

[6] Biotehniška fakulteta (1991): *Pedološka karta republike Slovenije. Sekcija Nova Gorica.* Ljubljana: Biotehniška fakulteta Univerze v Ljubljani.

[7] Bohte, Z. (1985): *Numerične metode.* Ljubljana: Društvo matematikov, fizikov in astronomov SRS, ZOTK Slovenije.

[8] Businger, J.A. (1975): Aerodinamycs of Vegetated Surfaces. In D.A. de Vries and N.H. Afgan (Eds.): *Heat and Mass Transfer in the Biosphere.* Washington D.C.: Scripta, 139 - 167.

[9] Campbell, G.S. (1985): *Soil Physics With Basic.* Amsterdam: Elsevier.

[10] Firdaouss, M., and Caussade, B. (1981): Numerical Simulation of Heat and Mass Transfer in Porous Materials. Proceedings of the 2nd International Conference Numerical Methods in Thermal Problems, Swansea, 269 - 276.

[11] Genuchten, M.Th. van (1980): A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. *Soil Sci. Soc. Am. J.*, **44**, 892 - 898.

[12] Haverkamp, R., and Vauclin, M. (1979): A Note on Estimating Finite Difference Interblock Hydraulic Conductivity Values for Transient Unsaturated Flow Problems. *Water Resour. Res.*, **15**, 181 - 187.

[13] Hillel, D. (1980): *Applications of Soil Physics.* New York: Academic Press.

[14] Hillel, D. (1982): *Introduction to Soil Physics.* New York. Academic Press.

[15] Horton, R., and Wierenga, P.J. (1984): The Effect of Column Wetting Soil Thermal Conductivity. *Soil Sci.*, **138**, 102 - 108.

[16] Jury, W.A, and Miller, E.E. (1974): Measurement of the Transport Coefficients for Coupled Flow of Heat and Moisture in a Medium Sand. *Soil Sci. Soc. Am. Proc.*, **38**, 551 - 557.

[17] Kimball, B.A., Jackson, R.D., Reginato, R.J., Nakayama, F.S., Idso, S.B. (1976): Comparison of Field-measured and Calculated Soil Heat Fluxes. *Soil Sci. Soc. Am. J.*, **40**, 18 - 25.

[18] Kluitenberg, G.J., and Horton, R. (1990): Analytical Solution for Two-Dimensional Heat Conduction beneath a Partial Surface Mulch. *Soil Sci. Soc. Am. J.*, **54**, 1197 - 1206.

[19] Mahrer, Y. (1982): A Theoretical Study of the Effect of Soil Surface Shape upon the Soil Temperature Profile. *Soil Sci.*, **134**, 381 - 387.

[20] Milly, P.C.D., and Eagleson, P.S. (1980): The Coupled Transport of Water and Heat in Vertical Soil Column under Atmospheric Excitation. Report No. 258, Department of Civil Engineering, Massachusetts Institute of Technology.

[21] Milly, P.C.D. (1982): Moisture and Heat Transport in Hysteretic, Inhomogeneous Porous Media: A Matric Head-Based Formulation and a Numerical Model. *Wat. Resour. Res.*, **18**, 489 - 498.

[22] Monteith, J.L., and Unsworth, M.H. (1990): *Principles of Environmental Physics*, Second Edition, London: Edward Arnold, Hodder and Stoughton.

[23] Mualem, Y. (1976): A New model for Predicting the Hydraulic Conductivity of Unsaturated Porous Mmedia. *Water Resources Research*, **12**, 513 - 522.

[24] Philip, J.R., and Vries, D.A. (1957): Moisture Movement in Porous Materials under Temperature Gradients. *Transactions of the American Geophysical Union*, **38**, 222 - 232.

[25] Saxton, K.E., Rawls. W.J., Romberger, J.S., Papendick, R.I. (1986): Estimating Generalized Soil-Water Characteristics from Texture. *Soil Sci. Soc. Am. J.*, **50**, 1031 - 1036.

[26] Virant, D. (1993): *Dinamično modeliranje vpliva padavin na fizikalne lastnosti tal.* Master of Science Thesis. Ljubljana: BTF, Agronomija.

[27] Vries, D.A. de (1958): Simultaneous Transfer of Heat and Moisture in Porous Media. *Transactions of the American Geophysical Union*, **39**, 909 - 916.

[28] Vries, D.A. de, and Afgan, N.H. (1975): *Heat and Mass Transfer in the Biosphere.* Washington D.C.: Scripta.

[29] Vries, D.A. de (1963): Thermal properties of Soils. In W.R. Wijk (Ed.): *Physics of plant Environment.* Amsterdam: North-Holland. 210-235.

[30] Vries, D.A. de, and Philip, J.R. (1986) Soil Heat Flux, Thermal Conductivity, and the Null-alignment Method. *Soil Sci. Soc. Am. J.*, **50**, 12 - 18.

[31] Wijk, W.R. van (1963): *Physics of Plant Environment.* Amsterdam: North-Holland.