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An evaluation of three numerical models used in simulations of the active layer and permafrost temperature regimes

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Abstract

Three numerical models (designated the Goodrich, Guymon/Hromadka, and Seregina models) used for calculations of the ground thermal regime which are based on different numerical methods and employ different treatments of freezing and thawing were compared with each other, with analytical solutions, and with measured temperature data. Comparisons of the models with the Neumann solution show differences generally less than 0.2°C between calculated temperatures using a wide range of time and depth steps. The Goodrich and Guymon/Hromadka models have been shown to predict temperature field dynamics reliably in the active layer and permafrost using small time and depth steps. However, comparisons of the models with each other using large time and depth steps and field data for the surface boundary condition showed significant differences between them (RMS deviations exceeding 1°C) and, in addition, the development of a non-physical feature (thaw bulb after freeze-up). Therefore, with large time and depth steps, the models cannot reproduce the temperature field dynamics in the active layer and permafrost. Consequently, agreement with the Neumann solution is necessary but not sufficient to qualify the models for calculations of real temperature fields. The Goodrich model requires a time step not longer than 1 h and depth step in the upper 1 m not larger than 0.02 m to reproduce the temperature regime with reasonable accuracy. However, the choice of optimum time and depth steps appears to be specific to the application. Using the Guymon/Hromadka model, similar accuracy can be obtained with a 1 h time step and 0.1 m space step within the upper 1 m depth or a 1 day time step and 0.01 m space step. However, the use of larger steps does not necessarily decrease the calculational time compared to the Goodrich model. For the case with unfrozen water present in the frozen soil, the results of calculations using the numerical models were compared with an analytical solution and were found to agree within 0.02°C.

Keywords: ? active layer, permafrost, modelling, unfrozen water

1. Introduction

Numerical modeling is one of the few methods which can provide information on the direction and consequences of global changes. Most of the current global circulation models (GCMs) are unable to reliably predict regional climatic changes resulting from a global-scale change (Hewitson, 1994), partly because of insufficient consideration of land–atmosphere interactions. In 'classic' GCMs only snow albedo was included but recent models take into

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account more complete information about surface conditions (snow cover characteristics, ground temperature, active layer thicknesses and characteristics, surface and ground hydrology) (Lynch et al., 1995).

Numerical modeling of the active layer and near-surface permafrost temperature field dynamics is also an important component of engineering design in northern regions particularly when properties change dramatically due to thawing of the permafrost (Osterkamp, 1982; Esch and Osterkamp, 1990; Osterkamp et al., 1997). For this reason, the accuracy of calculations of the active layer thicknesses and characteristics and the temperature regime of the active layer and near-surface permafrost become important.

A comprehensive review of numerical methods for ground thermal regime calculations was provided by Goodrich (1982b) and more recently by Alexiades and Solomon (1993).

In this paper, three models will be considered: a finite difference model (Goodrich, 1976, 1978a,b), designated the Goodrich model; a finite element model (Osterkamp and Romanovsky, 1996), which is a modified version of the Guymon and Hromadka (1977) and Guymon et al. (1984) model, designated the Guymon/Hromadka model; and a finite difference model (Seregina, 1989; Romanovsky et al., 1991b; Garagulya et al., 1995), designated the Seregina model.

Application of numerical methods for investigation of natural processes has to be justified by some kind of verification. Usually these verifications for thermal models are confined to comparison with analytical solutions for some simple cases with constant initial and boundary conditions (e.g. Neumann solution). Numerical models are not often verified using measured temperature data and are seldom compared to each other running with the same set of input data. In this paper, three models which employ different numerical methods and different treatments of freezing and thawing will be compared with each other, with analytical solutions, and with measured temperature data.

2. Model descriptions

All three models have been discussed in previous publications so only a brief description of the major characteristics of these models is given in this paper. The formulation of the Stefan problem in two dimensions is (Moiseenko and Samarsky, 1965):

$$C(T,x,y)\frac{\partial T}{\partial t} = \nabla[K(T,x,y)\nabla T],$$

$$(x,y,t) \in D, T \equiv T(x,y,t) \neq T_e \quad (1)$$

where $T(x,y,t)$ is the temperature field in the time–space domain $D = \{0 < x < l_1; 0 < y < l_2; 0 < t < t_1\}$, T_e is the temperature of the phase transition, C is the volumetric heat capacity, and $K(T,x,y)$ is the thermal conductivity. The initial and boundary conditions are:

$$T(x,y,0) = T_0(x,y) \quad (2a)$$

$$\left.\frac{\partial T}{\partial n}\right|_{x=0} = \left.\frac{\partial T}{\partial n}\right|_{x=l_1} = 0, \left.\frac{\partial T}{\partial n}\right|_{y=l_2} = g \quad (2b)$$

$$T(x,0,t) = \psi(x,t) \quad (2c)$$

where $(\partial)/(\partial n)$ is a normal derivative, g is the temperature gradient at the lower boundary of the domain D and $\psi(x,t)$ is the temperature change at the ground surface. The Stefan conditions at the phase boundary are:

$$T(x,y,t) = T_e \quad (3)$$

$$Q(x,y)\frac{\partial \Phi}{\partial t} = \{[(K\nabla T)|_{P+0} - (K\nabla T)|_{P-0}],$$

$$\nabla\Phi\} \quad (4)$$

with $P \in \Phi(x,y,t) = 0$, where $P \equiv P(x,y,t)$ is a point in an area D with coordinates x, y, t and $\Phi(x,y,t) = 0$ is the phase boundary equation in implicit form. $Q(x,y)$ is the latent heat of phase transitions, $P+0$ is an index that denotes the limiting value for a process that starts in a region with a higher enthalpy and proceeds towards a point on the phase front, $P-0$ is an index denoting a similar value but for a process starting in a region with lower enthalpy.

The Goodrich model is a one-dimensional finite difference model of heat flow in soils with phase changes, which includes the thermal effect of a snow cover with changing thicknesses and characteristics during the winter (Goodrich, 1976, 1978a,b, 1982a). It uses a central time finite difference equation for layered systems. The freezing and thawing interface is treated by a front tracking method which is capable of good accuracy for problems with all phase change at a fixed temperature. In case of the presence of two phase boundaries (during the freeze-up period), the heat flux between boundaries is assumed to be zero. This is justified by the fact that at a phase interface the heat flux from within the region bounded by two phase planes diminishes rapidly (in a few days) and the temperatures in this zone quickly approach the freezing point (Osterkamp and Romanovsky, 1997). The model was modified to include unfrozen water and temperature-dependent thermal soil properties using an apparent heat capacity method which is the same as in the Guymon/Hromadka model.

The temperature at the surface of the ground during the summer and at the surface of snow during the winter must be defined for the upper boundary condition. Input data also include the temperature or heat flux at the lower boundary as a function of time. The option to use linearized heat balance boundary conditions (Goodrich, 1982b) was also included. Snow cover thickness and density have to be described and an option allows density and thickness of the snow cover to be determined from the fresh snow thickness and density. Thermal properties of snow can be defined in the input data or calculated in the program. Calculational outputs are the dynamics of the ground and snow temperature fields.

The Guymon/Hromadka model is a two-dimensional finite element model for simulation of heat and moisture flow in unsaturated soils with phase change (Osterkamp and Gosink, 1991), which is a modified version of the Guymon and Hromadka (1977) and Guymon et al. (1984) model. The modified version includes two possibilities for calculating the freeze front position. One is a delta function formulation where latent heat releases or absorbs completely at a specified freezing point temperature with step function changes at the freeze front for the thermal properties. The second formulation provides for the possibility of unfrozen water in the frozen soils based on an apparent heat capacity approach with temperature-dependent thermal properties of the soils. This computer model was tested and identified as being physically realistic and appropriate for freezing soil conditions in Interior Alaska (Gosink et al., 1988). Temperature-dependent thermal properties were calculated using equations from Osterkamp (1987).

The Seregina model is a two-dimensional finite difference formulation of the equations for heat flow in nonhomogeneous soils with phase changes (Seregina, 1989; Romanovsky et al., 1991a,b; Garagulya et al., 1995). This model employs the enthalpy method where the heat capacity term in Eq. (1) is replaced by the time derivative of the enthalpy:

$$C_a(T, x, y)\frac{\partial T}{\partial t} = \frac{\partial H}{\partial t} \tag{5}$$

where C_a is an apparent heat capacity and H is enthalpy (Moiseenko and Samarsky, 1965; Alexiades and Solomon, 1993). The enthalpy and thermal conductivities are smoothed by polynomials of the first order. A completely implicit locally one-dimensional scheme is used to obtain a numerical solution to this problem with smoothed coefficients. Iterations are used to solve a discrete system of nonlinear grid equations at each time step. The solution from the previous time step is considered to be the initial approximation of the iterative process. The program cuts the time step in half in the case of iterative divergence.

3. Evaluation of models with no unfrozen water

All three models were compared with each other and with the Neumann solution for the case when the initial and boundary conditions were constant. The initial surface boundary condition was −5°C changing to a constant 10°C instantaneously in a step change for the period of calculations (1 year). Thermal conductivities in the frozen and thawed states were 1.97 W m^{-1} K^{-1} and 3.39 W m^{-1} K^{-1} and volumetric heat capacities were 2.9 MJ m^{-3} K^{-1} and 2.1 MJ m^{-3} K^{-1}, respectively. Volumetric moisture content was 0.4.

A sensitivity analysis of the models to the size of depth and time steps used two different sets of depth steps. One set consisted of 200 depth intervals from the surface to 100 m with the smallest step 0.1 m between 0 and 10 m depth and the largest step 2 m (between 60 and 100 m). The depth step increased gradually from 0.2 to 1 m between 10 and 60 m. Another set consisted of 200 depth intervals to the 16 m depth with the smallest step 0.01 m (between 0 and 1 m depth) and the largest step 1.0 m (between 12 and 16 m). Time steps were 1 day, 1 h and 7.2 min. Seven simulations were conducted (simulations I through VII in Table 1). Results of the simulations were the daily mean temperatures during 1 year of simulation (365 rows) at 16 different depths (within the upper 1 m the output interval was 0.1 m, between 1 m and 2 m, 0.2 m, and the last depth in the output file was 2.5 m). Results of comparisons of the root mean square (RMS) deviations between each pair (5840 components of the output matrices for any two models) of calculated daily mean temperatures during the whole year in the depth interval between 0 and 2.5 m are shown in the Table 2.

Table 2 shows RMS deviations of less than 0.13°C between calculated temperatures using different models, time and space steps except for the results involving simulation III where the differences were 0.21° to 0.29°C. Moreover, the largest deviations in simulations I through IV and especially simulation VII occurred during the first 10 days of calculations. These results would appear to justify the use of the models for calculating the thermal regime of the active layer and permafrost. However, the following will show that this conclusion may be premature in some cases.

Calculations using measured daily mean ground surface temperatures (Romanovsky and Osterkamp, 1995) for 1989 near Franklin Bluffs in the Prudhoe Bay region, Alaska, which changed rapidly with time, were used to test the models for application to field data. Thermal properties and moisture contents of the soils were the same as in the first series. This combination of input data provided an active layer thickness of 1.4 m. Seven simulations (VIII through XIV) were conducted using different models and different time and depth steps (Table 1). The values of RMS deviations between these simulations were calculated as for the first series and the results are shown in Table 3. Calculated RMS deviations were significantly larger than those shown in Table 2. The values for simulations VIII and for XII are unaccept-

Table 2
Root mean square deviations between each pair of calculated daily mean temperatures (in °C) in simulations I through VII and using the Neumann solution

Simulations	I	II	III	IV	V	VI	VII	Neumann
I		0.12	0.21	0.12	0.10	0.11	0.12	0.10
II			0.28	0.03	0.04	0.04	0.04	0.04
III				0.29	0.26	0.27	0.28	0.26
IV					0.03	0.02	0.03	0.03
V						0.01	0.03	0.01
VI							0.02	0.01
VII								0.03
Neumann								

Table 3
Root mean square deviations between each pair of calculated daily mean temperatures (in °C) in simulations VIII through XIV

Simulations	VIII	IX	X	XI	XII	XIII	XIV
VIII		1.41	1.32	1.26	0.62	1.17	1.23
IX			0.42	0.34	1.33	0.79	0.36
X				0.21	1.42	0.48	0.25
XI					1.34	0.33	0.22
XII						1.23	1.37
XIII							0.35
XIV							

Table 1
Models, time steps and minimal depth steps used in each of fourteen simulations

Simulations	Model	Time step	Minimal depth step/maximal depth (m)
I and VIII	Guymon/Hromadka	1 day	0.1 /100
II and IX	Guymon/Hromadka	1 h	0.1 /100
III and X	Guymon/Hromadka	1 day	0.01/16
IV and XI	Guymon/Hromadka	1 h	0.01/16
V and XII	Goodrich	1 h	0.1 /100
VI and XIII	Goodrich	7.2 min	0.01/16
VII and XIV	Seregina	1 h	0.01/16

ably large (more than 1°C). Moreover, the behavior of the calculated values in these two simulated temperature fields (VIII and XII) show unrealistic features where, after freeze-up, a 'thaw bulb' appeared at the permafrost surface and moved downward during the following 2 months. However, the Goodrich and Guymon/Hromadka models have been shown to predict active layer and permafrost temperatures reliably when using small time and depth steps (Romanovsky and Osterkamp, 1997). It is concluded that, using large time and space steps, the models cannot reproduce the temperature field dynamics in the active layer and permafrost.

Simulation V in the first series, which was the analogy for XII (Table 1), showed the best agreement with the Neumann solution. Thus, agreement with the Neumann solution is a necessary condition but not a sufficient one to justify the use of the models for calculating real temperature fields in case of rapid temperature changes at the ground surface.

The differences between the Guymon/Hromadka and Goodrich models for small time and space steps (XI and XIII) appeared after the start of active layer freezing from the ground surface downwards. Deviations in RMS values between these two simulations during the first 260 days is only 0.03°C with a maximum difference of 0.15°C for all depths. Additional calculations using the Goodrich model (results not included in the Table 3) with different time and depth steps showed, that to predict the thermal regime of the active layer and permafrost in real situations with reasonable accuracy (within 0.3–0.4°C), the time step should not be longer than 1 h and depth step in the upper 1 m not larger than 0.02 m. Using the Guymon/Hromadka model, this accuracy can be reached with 1 h time steps and 0.1 m depth steps within the upper 1 m depth or 1 day time steps and 0.01 m depth steps. However, the possibility of using larger steps does not necessarily decrease the time of calculations compared to the Goodrich model. Computational time is approximately equal in these two cases, because the two-dimensional Guymon/Hromadka model generally is more time consuming than the one-dimensional Goodrich model (for the same time and depth steps).

Additional calculations using the Goodrich model show that the size of acceptable time and depth steps for this model depends strongly on the rate of active

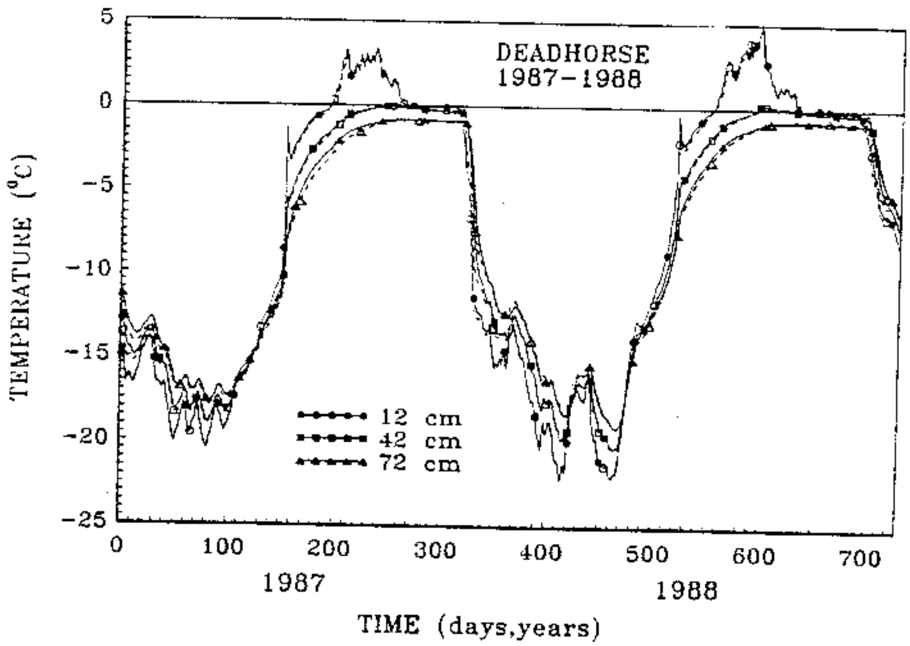

Fig. 1. Comparison between calculated temperatures (dashed lines and open symbols) and measured temperatures (solid lines and filled symbols) at three depths (0.12, 0.42 and 0.72 m) during 1987 and 1988 at the Deadhorse site in the Prudhoe Bay region, Alaska.

layer thawing which is a function of the thermal parameters of the soils (thermal conductivity and latent heat of the soil moisture) and the temperature regime at the ground surface. In some calculations with the above input data, even 1 h time steps and 0.1 m depth steps were too large to obtain physically reasonable results. At the same time, calculations using West Dock site conditions (active layer thickness between 0.2 m and 0.4 m) showed that the results of simulations with 7 min time steps and 0.01 m depth steps could be reproduced to within 0.1°C with 3 h time steps and 0.1 m depth steps. Therefore, the choice of optimum time and depth steps appears to vary for each case so that special care is necessary in applying the model.

An additional constraint on the Goodrich model is that it can become unstable when more than two phase boundaries are present. For example, in the case of a freezing active layer there are two moving phase boundaries separated by a isothermal region. However, a short period of thaw at the ground surface followed by refreezing introduced two more phase boundaries near the ground surface. This sometimes caused the model to become unstable although a new version being developed may solve this problem (L.E. Goodrich, pers. commun.).

Results of calculations using the Guymon/Hromadka and Goodrich models were compared with each other and also with the measured temperature data in the active layer and permafrost at the West Dock site in the Prudhoe Bay region, Alaska, in 1987 (Romanovsky and Osterkamp, 1997). It was found that, for the case of small time and depth steps (the same as in XI and XIII), the results of calculations of the daily temperatures using both models differed by only 0.02°C for the whole year (1987) for 18 depths from 0.02 to 0.87 m, except for 1 day just after freeze-up, when the difference reached 0.35°C at the depth of 0.17 m. The RMS deviation between the results of these two

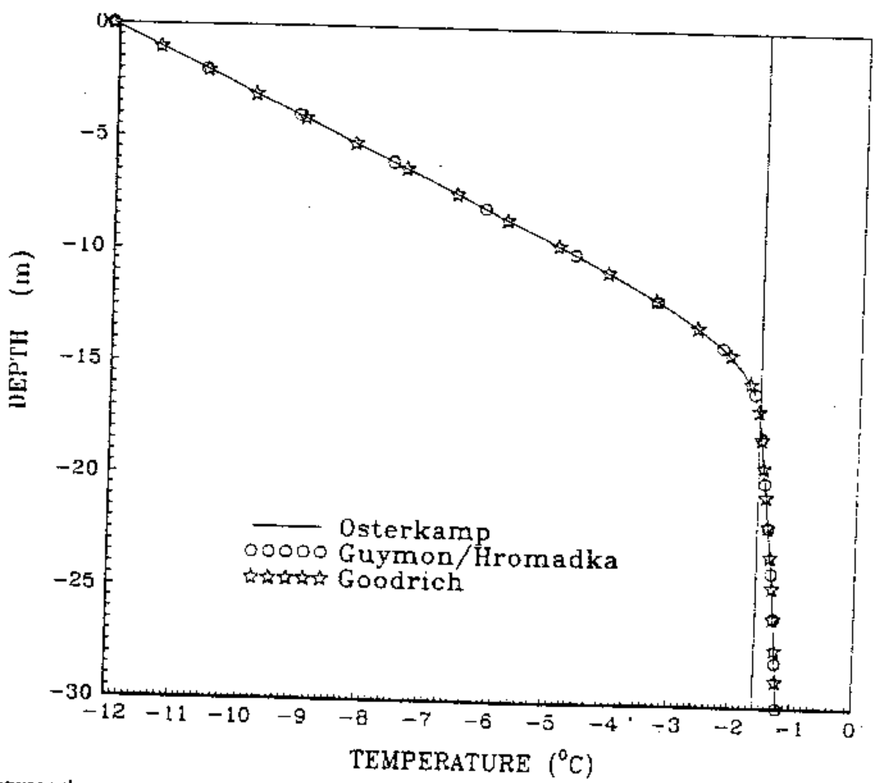

Fig. 2. Comparison between the temperature profiles calculated using the Guymon/Hromadka and Goodrich models (open symbols) and an analytical solution from Osterkamp (1987) (solid line) after 10 years when unfrozen water was present in the frozen soil.

models for the whole year and for all depths was 0.012°C.

Fig. 1 shows an example of a comparison between calculated temperatures, using the Guymon/Hromadka model (dashed lines and open symbols), and measured temperatures (solid lines and filled symbols) at three depths (0.12, 0.42 and 0.72 m) during 1987–1988 at the Deadhorse site in the Prudhoe Bay region, Alaska. This comparison shows differences between calculated and measured data of 0.1° to 0.2°C during the whole year, except for 30 to 40 days in the Spring (differences up to 0.5°C) and during freeze-up and the following cooling period, when deviations were more than 2°C. These large errors appear to be associated with the presence of a significant amount of unfrozen water in the cooling active layer after freeze-up (Osterkamp and Romanovsky, 1997). Additional examples of the comparison between calculated and measured temperature data can be found in Romanovsky and Osterkamp (1997).

4. Comparison of the models with unfrozen water

The Guymon/Hromadka model and a modified version of the Goodrich model (to include the effects of unfrozen water) were compared with an analytical solution to the problem of freezing and thawing of soils containing unfrozen water or brine (Osterkamp, 1987). The weighted geometric mean equation (Lachenbruch et al., 1982) was used to calculate the temperature-dependent thermal conductivity $K(T)$. Apparent heat capacity, $C_a(T)$, and other thermal properties and parameters were taken from Osterkamp (1987). The mass fraction of unfrozen water was calculated using (Osterkamp and Romanovsky, 1997):

$$w_u(T) = A|T - E|^B + F \tag{6}$$

where T is temperature in degrees Celsius and A, B, E and F are empirical constants ($A = 0.3795$, $B = -0.7790$, $E = 0$, and $F = 0$).

In the apparent heat capacity, the latent heat term:

$$L\frac{\partial \theta_u}{\partial T} = -\frac{\rho_b}{\rho_u} L A B |T - E|^{B-1}. \tag{7}$$

The initial temperature was assumed to be −1.0°C and the equilibrium temperature of the phase transitions was −1.6°C. A constant surface temperature of −12.1°C was applied instantaneously and maintained over the whole period of calculations. Fig. 2 shows the results of these calculations for each model and the analytical solution after 10 years of freezing. All three temperature profiles are within 0.02°C of each other. Since the Guymon/Hromadka model has been tested and found to be satisfactory for interpreting field data when unfrozen water was present (Osterkamp and Romanovsky, 1997), this suggests that the modified version of the Goodrich model can also be used for these cases. Examples of comparisons of the calculated and measured temperature data can be found in Osterkamp and Romanovsky (1997).

5. Conclusions

Three numerical models for ground thermal regime calculations based on different numerical methods and different treatments of freezing and thawing were compared with each other, with analytical solutions, and with measured temperature data. Comparisons with the Neumann solution show RMS deviations between the models and between simulations with the same models of less than 0.3°C and, typically, less than 0.13°C between calculated temperatures using a wide range of time and space steps. However, when using field data with rapidly changing temperatures at the ground surface and with large time and space steps, the models disagreed with each other and developed a non-physical feature (thaw bulb after freeze-up). Using small time and depth steps, the Goodrich and Guymon/Hromadka models predict active layer and permafrost temperatures reliably. Therefore, it is concluded that they cannot accurately reproduce the temperature field dynamics in the active layer and permafrost when using large time and depth steps. Thus, agreement with the Neumann solution is a necessary condition but not a sufficient one to justify the use of the models in calculations of real temperature fields.

With the Goodrich model, time steps not longer than 1 h and depth steps in the upper 1 m not larger than 0.02 m have to be used to reproduce the thermal regime with reasonable accuracy. However, the choice of optimum time and depth steps appears to be specific to the application. Using the Guymon/Hromadka model, the same accuracy can be obtained with 1 h time steps and 0.1 m space steps within the upper 1 m depth or 1 day time steps and 0.01 m space steps. However, the use of larger steps does not necessarily decrease the time of calculations compared to the Goodrich model.

When unfrozen water is present in the frozen soils, the results of calculations using a modified Goodrich and the Guymon/Hromadka models were compared with an analytical solution and found to agree within 0.02°C.

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