2.24 Temperature and heat transport model

The following theoretical derivations were mainly obtained from Ronald Daanen, University of Alaska, Fairbanks, who supported the development of the heat transfer model.

The movement of heat in soils follows two principles: Conservation of heat (first law of thermodynamics) and Fouriers Law or the heat flux (second law of thermodynamics).

The conservation of heat means, that the change of the internal energy of a system is only due to energy added to or removed from the system and by work done by the system.

$$dU = \delta Q - \delta W \qquad \textbf{(2.24.1)}$$

where dU is the change in internal energy, δQ is the net balance of energy fluxes and δW is the work done by the system (all units in Joule). We can neglect the term δW, since we deal with a system consisting only of solid and liquid materials, and no external pressure changes are taken into account. Equation (2.24.1) can therefore be simplified into

$$dU = dQ \qquad \textbf{(2.24.2)}$$

The energy content of a soil can change over time due to temperature variations. The heat flux through the soil matrix (conduction) can be a large component of the ground heat transfer. Note that non-conductive heat transfer by flow of water and water vapour can be a dominant form of heat transfer in cold climates (Kane et al. 2001). The user can choose to simulate heat transfer by advection starting with WaSiM version 9.00.13 (October 2012).
For the process of heat transfer, the left and right side of Eq. (2.24.2) can be written as:

$$C(T)\cdot\frac{\partial T}{\partial t} = \nabla\cdot\lambda(T)\cdot\nabla T + q_s \qquad \textbf{(2.24.3)}$$

where $C(T)$ is the temperature dependent heat capacity of the soil, $\partial T/\partial t$ is the temperature change in time, $\lambda(T)$ is the temperature dependent thermal conductivity. The Nabla operator ∇ defines the temperature gradient (of the scalar field T) as ∇T and the divergence of the vector field $\lambda(T)\nabla T$ as $\nabla\cdot(\lambda(T)\nabla T)$; q_s is the source/sink term, i.e. heat that enters or leaves the system by advective transport due to water fluxes (later, that term will also be used for defining a lower boundary condition as known constant heat flux). Eq. (2.24.3) could also be written as

$$C(T)\cdot\frac{\partial T}{\partial t} = \mathrm{div}\left(\lambda(T)\cdot grad\ T\right) + q_S \qquad \textbf{(2.24.4)}$$

(Note the resemblance to the water flux in the Richards approach). This differential equation must be integrated to be used within the finite differences approach of the Richards equation. The discrete form of Eq. (2.24.4) applied to a 1D-vertical soil profile can be written as:

$$\rho\cdot V\cdot C(T)\cdot\frac{\Delta T}{\Delta t} = \lambda(T)\cdot\frac{A}{L}\cdot\Delta T = Q_{\mathrm{in}} - Q_{\mathrm{out}} + q_S \qquad \textbf{(2.24.5)}$$

where ρ is the density of liquid water (we will use 1000 Kg/m^3 here), V is the elementary volume (let's assume that it is 1 m^3), A is the elementary area (let's assume as 1 m^2), L is the elementary length (we assume 1 m here), Q_{in} and Q_{out} are the heat fluxes through the upper and the lower boundary of the elementary volume.

Before breaking down the single terms in Eq. (2.24.5), it should be noted that the heat transfer in a partly ice and/or water saturated soil (which means that there can be water, air and ice at the same time besides the soil matrix particles) is a little bit more complex than the heat transfer through a monolithic block of matter:

1. The phase change of water to ice and vice versa is a process depending on the soil porosity characteristics. Usually, the phase change mainly takes place between -10°C and 0°C, with water in the smallest pores freezing last (and thawing first) and water in the biggest pores freezing first (and melting last). In silty soils, the phase change reaches down to deeper temperatures (e.g. 90% ice, 10% water at -5°C possible, see Williams (1964)) than in sandy soils or even in peat (moor), where 90% of the water is already frozen at -0.5 to -1°C (Spaans (1996), Figure 1 and Nagare et al. (2011), Figure 5)
2. The thermal conductivity, λ, is also dependent on the ice or water content of the soil and is thus, indirectly dependent on temperature T. In fact, λ is an integrated parameter for the given soil's characteristics as the distribution of the individual components (soil matrix, water, ice, and air) should be taken into account.
3. The same is true for the heat capacity $C(T)$, where the soil matrix, ice, and water (we neglect air here) all have individual specific heat capacities. In addition, the phase change of water to ice, and vice versa, with its latent heat, L_h = 334 KJ/Kg, leads to changes in the effective heat capacity at any given temperature between 0°C and -10°C as, depending on the soil type, water can exist in soils below 0°C.
4. Changes is the distribution of water and ice, the effective thermal conductivity and the temperature dependent heat capacity (due to latent heat change) can be described using the same parameterization scheme as for the soil hydraulics properties: the van-Genuchten-parameterization. So the parameters m, n and α used for describing $k(\Theta)$ and $h(\Theta)$ can also be used in much the same way to describe the thermal properties.

Having said this, the following equations will describe the development of the soil heat transfer functions from its basic parameters. Note that the following algorithms will be applied iteratively for each numerical soil layer, side by side with the Richards-equation since both processes affect each other. Consequently, the soil heat transfer model is integrated into the soil model and could take a considerable amount of computing time depending on soil layer thickness heat gradients, thermal conductivity etc.

The first step in calculating 1D heat transfer by conduction is to estimate the fraction of ice and water, i.e. the relative saturation, S_E. A value of 1 means that there is only liquid water, while a value of 0 means that there is only ice. Note that an S_E value of 1 doesn't mean that the entire pore volume is filled with water. S_E only refers to the total amount of water that is present in the soil, which, in turn, is calculated by the mass transport equation following the Richard's approach.

Estimation of the relative saturation, S_E

$$
\begin{aligned}
S_E &= \left(\frac{1}{1+\left(\alpha\cdot\left|f\cdot T_{eff}\right|\right)^n}\right)^m \qquad &\text{for } T\le 0\,°\text{C} \\
S_E &= 1 &\text{for } T>0\,°\text{C} \\
&\text{with } T_{eff}=\left(T+T_{Shift}\right)
\end{aligned}
\qquad \textbf{(2.24.6)}
$$

where S_E is the relative fraction of liquid water of the total soil moisture; n, m and α are the van-Genuchten-Parameters as used in the Richards equation; T is the soil temperature in °C; and f is the solution of the Clapeyron-equation assuming zero ice pressure (333 KJ/Kg / 273.15 K at or near 0°C = 1.22 KJ/(Kg·K)). For temperatures above 0°C, S_E is always 1, whereas for temperatures below -10°C the value of S_E is assumed to be 0. The latter assumption is to reduce computational demand. Very fine grain soils may still contain water below -10°C, but the fraction is negligible to any thermal and hydraulic transport process at the timescales of typical WaSiM applications.

The temperature shift expressed by T_{shift} accounts for unsaturated conditions by shifting the temperature dependence of S_E to lower temperatures, depending on the hydraulic pressure (which in turn depends on the relative water saturation of the pore volume). The algorithm to estimate the temperature shift is explained later when dealing with the latent heat change (see equation (2.24.10) and figure 6).

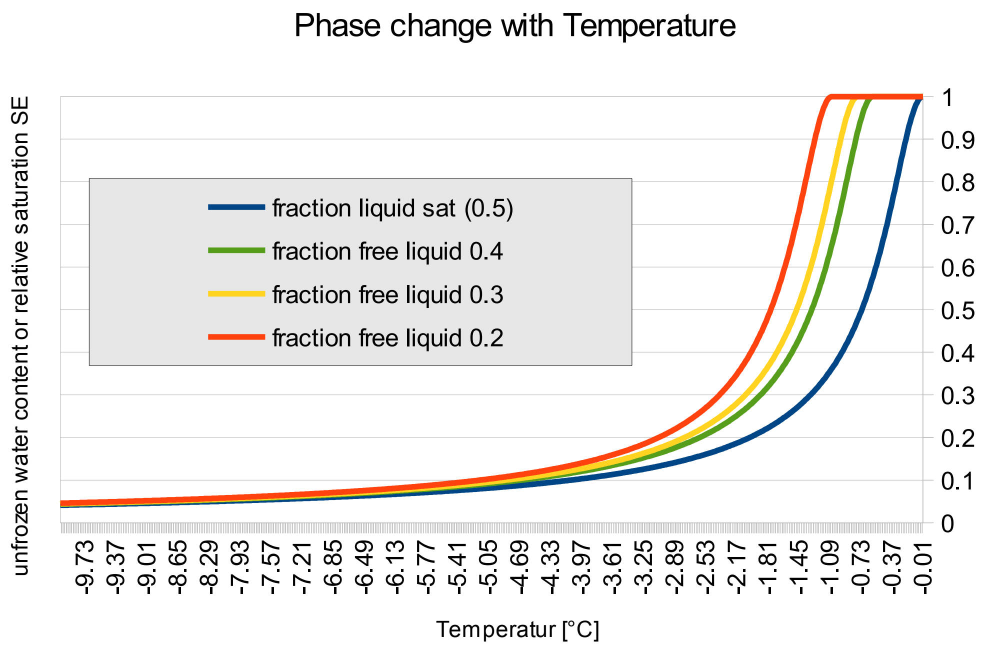

Figure 1: Change in the fraction of liquid water, $S_{E,}$ during temperature change in a sandy loam soil (alpha=2, n=2, m=0.5).

Figure 1 shows the fraction of liquid water with temperature change computed for a silty soil (van-Genuchten parameters m =0.5 n =2 and α = 2, saturation water content 0.5, residual water content 0.1). The green, yellow and red curves show the relative saturation values for unsaturated soild with different water contents (see explanations for equation (2.24.10) below for details).

Estimation of the effective thermal conductivity, $\lambda(T)$

The next step is to estimate the effective thermal conductivity which depends on the relative fractions of liquid water content, ice content (and thus on relative saturation S_E), dry soil and air content:

$$\lambda_{eff}=(\varphi-\Theta)\cdot\lambda_a+(\Theta+\theta_{ds})\cdot\lambda_{ds}^{\theta_{ds}/(\Theta+\theta_{ds})}\cdot\lambda_l^{\theta_l/(\Theta+\theta_{ds})}\cdot\lambda_{ice}^{\theta_{ice}/(\Theta+\theta_{ds})} \qquad \textbf{(2.24.7)}$$

where λ_{eff} is the effective thermal conductivity in J/(m·s·K); φ is the porosity, Θ is the total water content (ice and water), $\lambda_{a,\, ds,\, l,\, ice}$ is the thermal conductivity of air, dry soil, liquid water and ice, $\theta_{ds,\, l,\, ice}$ is the dry soil, liquid water and ice content as relative volume fractions. (the default value of λ_a is set to 0.0262 J/(m·s·K), λ_{ds} = 0.58 J/(m·s·K) - unless this parameter is defined in the soil table), λ_l = 0.5562 J/(m·s·K) and λ_{ice} = 2.33 J/(m·s·K). Note: θ_l can be expressed by $S_E \cdot \Theta$ (liquid fraction on water content or unfrozen soil water) and $\theta_{ixe} = (1-S_E)\cdot\Theta$.

Note that we will make no difference whether the soil is completely saturated with water or not. All soils have a certain amount of soil water, and if there were no water at all in the soil, the connecting points between soil grains were so small, that the heat transfer will become extremely restricted – so the water improves the conduction massively, no matter if the soil is partly or fully saturated. The thermal conductivity of non-dry soil is thus much more like the conductivity of water or ice, so an effective value may be used here.

The effective thermal conductivity during temperature change (i.e. change in the fraction of liquid water) for a sandy loam soil is presented in figure 2. The van Genuchten parameters (*m, n* and *α)* used to calculate the fraction of liquid water are identical to those used in figure 1 with $\lambda_{soil,dry}$ = 0.58 J/(m·s·K), λ_{water} = 0.5562 J/(m·s·K) and λ_{ice} = 2.33 J/(m·s·K).

The different graphs show the effect of different total water contents Θ_{rel} (blue: saturated soil with Θ=0.5). As can be seen for saturated conditions (relative water content Θ_{rel} = 1), the thermal conductivity at 0°C (and warmer) is the weighted average of the dry soil thermal conductivity and the thermal conductivity of water, whereas the deeply frozen soil (near –10°C) has an almost constant value, which is mainly represented by the weighted average of dry soil and ice thermal conductivities.

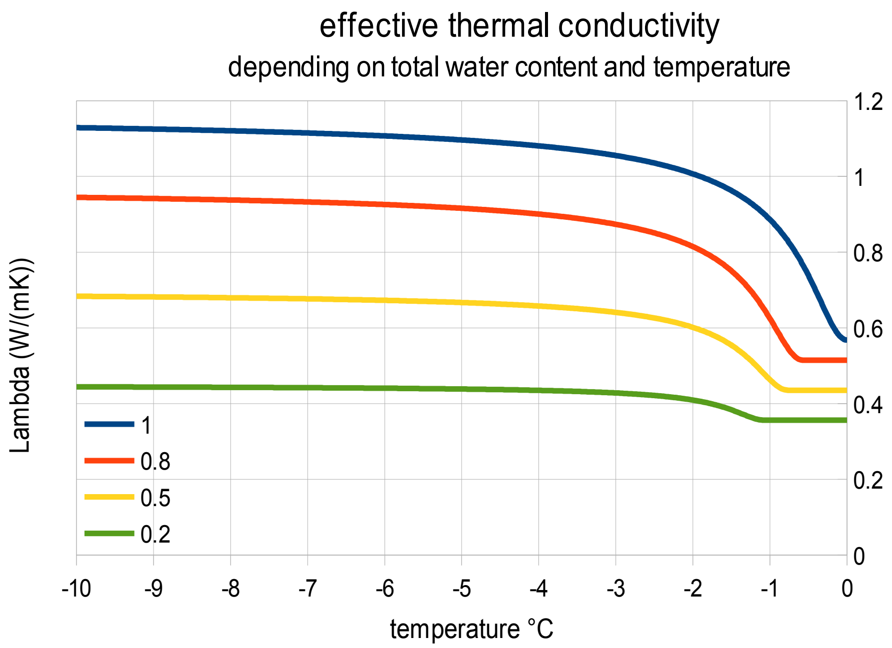

Figure 2: Effective thermal conductivity plotted against soil temperature.

Estimation of the effective hydraulic conductivity

The effective hydraulic conductivity can be calculated using different approaches. The most simple approach would be to linearly interpolate between the saturated frozen and the saturated thawed hydraulic conductivities k_f and k_t:

$$k(T) = S_E \cdot k_t + (1 - S_E) \cdot k_f \qquad \textbf{(2.24.8a)}$$

where $k(T)$ is the effective hydraulic conductivity in m/s; k_t is the (thawed soil) hydraulic conductivity for S_E = 1 and k_f is the frozen hydraulic conductivity when all pores are filled with ice ($S_E \approx 0$). The frozen saturated hydraulic conductivity, k_f, can be defined as a parameter in the soil table (default is set to 10^{-8} m/s).

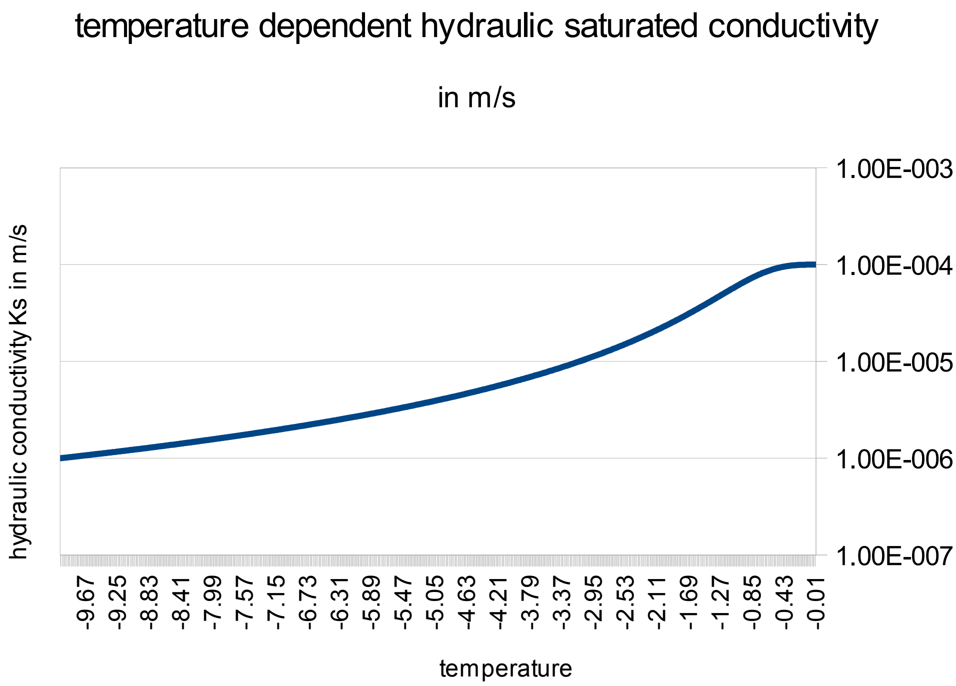

Figure 3: Effective thermal conductivity based upon Eq. (2.24.8a)

The effective hydraulic conductivity decreases with an increasing fraction of ice, i.e. a decreasing S_E-value (Figure 3). The effective hydraulic conductivity changes with several orders of magnitude as the soil freezes/thaws. However, Eq. 2.24.8a does not result in the exponential response in effective hydraulic conductivity as has been measured for freezing/thawing mineral and organic soils (see Zhang et al. 2010). Accordingly, a modified exponential function could be applied to calculate the effective hydraulic conductivity (Figure 4):

$$k(T)=e^{S_E\cdot\ln(k_t(\Theta))+(1-S_E)\cdot\ln(k_f)} \quad \textbf{(2.24.8b)}$$

The resulting graph (Figure 4) is more independent of the van-Genuchten α or n, since the error on the lower end of the temperature scale is now almost completely eliminated. This example uses a moderate frozen hydraulic conductivity of 10^{-9} m/s.

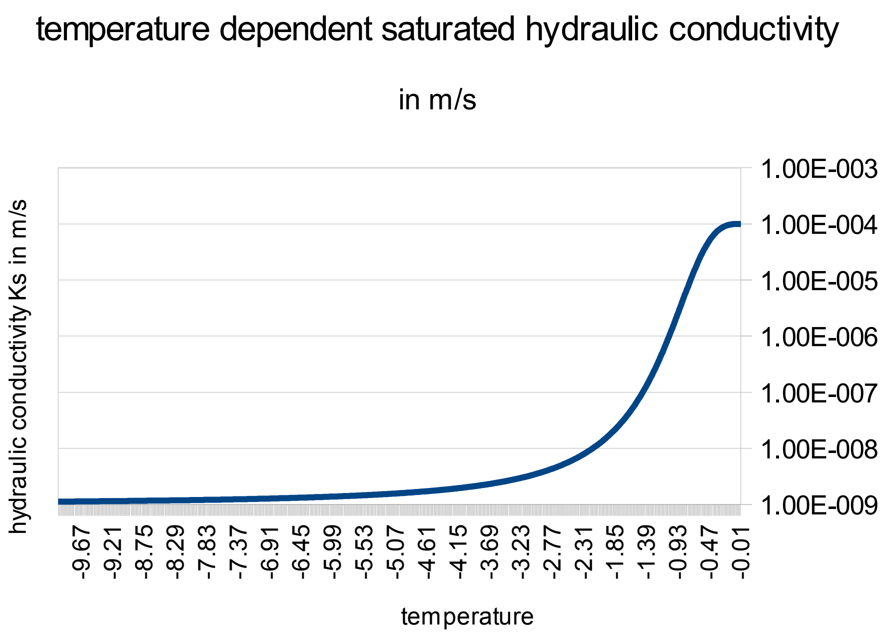

Figure 4: Effective hydraulic conductivity using an exponential function (Eq. 2.24.8b).

However, when soils freeze, they are not always saturated. Especially for peat, the hydraulic conductivity is not as small as equation (2.24.8b) suggests, since water can infiltrate into the largest pores quite good. The hydraulic conductivity must take into account all soil parameters as well as temperature dependent effects, e.g. by using the relative water saturation S_E.

Therefore, WaSiM uses an approach that again builds on the similarity between the parametrization of hydraulic and thermal conductivities in soils.

$$k(T,S_{min})=k_{sat}\cdot k_{rel}(T,S_{min})$$
$$k_{rel}(T,S_{min})=S_{min}^{0.5}\cdot\left(1-\left(1-S_{min}^{n}\right)^{m}\right)^{2} \qquad \textbf{(2.24.8c)}$$
$$\text{with } S_{min}=\min\left(S_E,S_R\right) \quad \text{and} \quad S_R=(\Theta_{sat}-\Theta_{res})/(\Theta_{act}-\Theta_{res})$$

Where $k(T,S_{min})$ is the effective hydraulic conductivity in m/s; k_{sat} is the saturated hydraulic conductivity in m/s; m, n and α are the van-Genuchten-parameters as used in the Richards equation, S_E and S_R are the unfrozen water fraction of the soil water and the filled relative pore volume, respectively; Θ_{sat}, Θ_{res} and Θ_{act} are the saturated, the residual and the actual water content of the soil, resp. This is basically the same as in equation (2.14.5), except that here the relative free water content with respect to the pore volume can be replaced by the unfrozen water content for lower temperatures.

This approach results in specific unsaturated hydraulic conductivities for each saturation level, as is shown in figure 5. It compares the unfrozen water content of the soil S_E to the relative water saturation value from the Richards-equation set S_R. As long as the unfrozen water content of the soil S_E is higher than the value of S_R, the value of k_{rel} follows the van-Genuchten parameterization of the Richards approach. When the soil freezes, S_E decreases until it eventually becomes smaller that S_R. Now, S_E is the limiting factor for the hydraulic conductivity.

The important thing about this approach is, that the infiltration into the uppermost unsaturated layer is always possible with a higher infiltration rate than given by the k-value (since otherwise a dry soil would never wet up). So once the uppermost layer contains some water, the hydraulic conductivity of that layer rises as well until it can supply some water to the lower next layer – as long as the water will not freeze and thus block the pores for more infiltrating water.

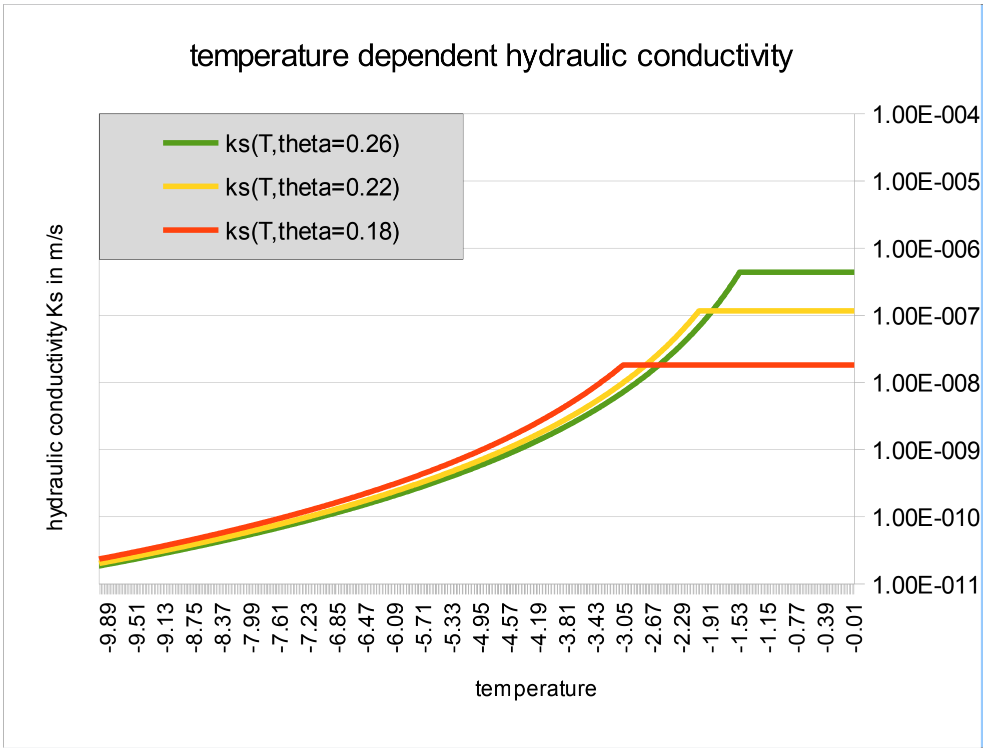

Figure 5: Effective unsaturated hydraulic conductivity using an exponential function and a variable ks-value based on equation (2.24.8c)

Figure 5 shows a shift of the temperature dependent hydraulic conductivities to slightly higher values for soils with less total water (filled pores). This is an effect of the higher fraction of liquid water (unfrozen water S_E), since the water in the smallest pores freezes last and thus there may still be some minor water flux possible, although the hydraulic conductivity is very soon reaching extremely low values with falling temperatures.

Note: the example in figure 5 uses the same van-Genuchten parameters (n=2, α=2 m^{-1}) as in figure 4 and that no parameter is needed for the frozen conductivity as was the case for the other methods above.

Estimation of the effective heat capacity, *C*(*T*):

The heat capacity, $C(T)$, is by definition the amount of energy per unit volume (m^3) required to raise the temperature by 1 K. The effective heat capacity can be calculated by knowledge of the volume fractions of soil (mineral or organic), water, ice, and air, and their respective specific heat capacity and density (we neglect the air here):

$$C(T)=\rho_{soil}\cdot C_{\text{soil,dry}}+\rho_l\cdot\Theta_{\text{act}}\cdot\left(S_E\cdot C_t+(1-S_E)\cdot C_f\right)+\frac{\partial E}{\partial T} \qquad \textbf{(2.24.9)}$$

where $C(T)$ is the effective heat capacity in J/(m^3·K),
C_t the specific heat capacity of liquid water is a material "constant" given by 4187 J/(Kg·K),
C_f the specific heat capacity of ice is given by about 2000 J/(Kg·K) (depending on temperature between 1940 J/(Kg·K) at -20 °C and 2090 J/(Kg·K) at 0 °C),
$C_{\text{soil,dry}}$ the specific heat capacitiy of dry soil, which is a material constant in J/(Kg·K)

	that must be defined as a parameter in the soil table (default = 800 J/(Kg·K)),
ρ_{soil}	the dry density of soil in kg/m^3 (must also be defined in the soil table, default = 1500 Kg/m^3)
ρ_l	density of (liquid) water at 0 °C ≈ 1000 Kg/m^3
Θ_{act}	actual water content in m^3/m^3 following the Richards-approach

The energy change $\partial E / \partial T$ (in J/(m^3·K)) can be described using the van-Genuchten-parameters:

$$\frac{\partial E}{\partial T} = L_f \cdot \rho_l \cdot (\Theta_{act} - \Theta_r) \cdot m \cdot n \cdot \alpha \cdot f \cdot \left(-\alpha \cdot f \cdot T_{eff}\right)^{(n-1)} \cdot \left(1 + \left(-\alpha \cdot f \cdot T_{eff}\right)^{n}\right)^{(-m-1)} \quad \text{in } \frac{\text{J}}{\text{m}^3 \cdot \text{K}} \qquad \textbf{(2.24.10)}$$

$$\text{with } T_{eff} = \left(T + T_{shift}\right) \quad \text{for } T < 0\,°\text{C}$$

where

L_f	latent heat of fusion for ice = 334000 J/Kg
ρ_l	density of (liquid) water at 0 °C ≈ 1000 Kg/m^3
Θ_{act}	actual water content in m^3/m^3
Θ_r	residual water content in m^3/m^3
m,n,α	van-Genuchten parameter as used in the soil table
f	factor connected to the solution of the Clapeyron-equation in m/K. Literature suggests different values (123 m/K in Daanen and Nieber (2009), (-)1.8 m/K in Grant (2000). We will use rather values in the range of 1.22 or 1.8 m/K, since higher values shift the freezing point even for soils with a very small fraction of liquid water extremely near to the 0 °C line (e.g. -0.02 °C for f = 123)
T	Temperature of the modelled volume (assuming even distribution for water, soil matrix, ice and air in a numeric layer)
T_{eff}	The effective temperature due to partly unsaturated conditions, depending on the actual volumetric water content
T_{shift}	Temperature shift for starting freezing due to higher pore pressure for unsaturated conditions

Figure 6 shows the change in energy (latent heat) with a given change in temperature (note that δE/δT = 0 for $T > 0$°C). The graph represents a differential expression so the resolution of the x-axis (0.01 K) has to be taken into account. If the temperature of a volume of ground changes by 0.01 K, then the change in energy of that volume is presented by the value on the y-axis. Energy is lost from the volume if the ground freezes, and gained by the volume if the ground thaws (ice melt). For example, for a temperature change from -0.5 °C to -0.51 °C (freezing), the amount of energy released is 997060 J/m^3 (Θ_s = 0.5 and Θ_r = 0.1, n=2, α=2). The entire area below the graph, which is the total energy that would be required to thaw the soil, should result in a latent heat of $L_f \cdot \rho_l \cdot (\Theta_s - \Theta_r)$ = 334 KJ/Kg · 1000 Kg/m3 · (0.5 – 0.1) = 133.6 MJ/m^3 for saturated conditions (blue graph), whereas the area below red graph has a reduced value that corresponds to the water content, in this case 0.2·133.6 MJ/m^3 = 26.72 MJ/m^3.

Note that for saturated soils the integral of the part of equation (2.24.10) after the term (Θ_{act}-Θ_r) will give the result of 1.0 for ideal conditions (with integration limits from -∞ to 0), but practical applications (with integration limits from -10°C to 0°C) will usually result in slightly smaller values like 0.99 or so (for clay this may even be considerably less at about 0.6 only).

The change in effective heat capacity is at its largest when the change in water/ice fraction is high (slope of the phase change diagram is steepest), which coincides with the largest latent heat change (Figure 7). Water has a higher heat capacity than ice. The maximum slope of phase change and the maximum change in latent heat is at about -0.57 °C, whereas the maximum heat capacity is already at approx. -0.25°C for this specific soil, since the frozen part of the soil water reduces the overall heat capacity due to its lower heat capacity.

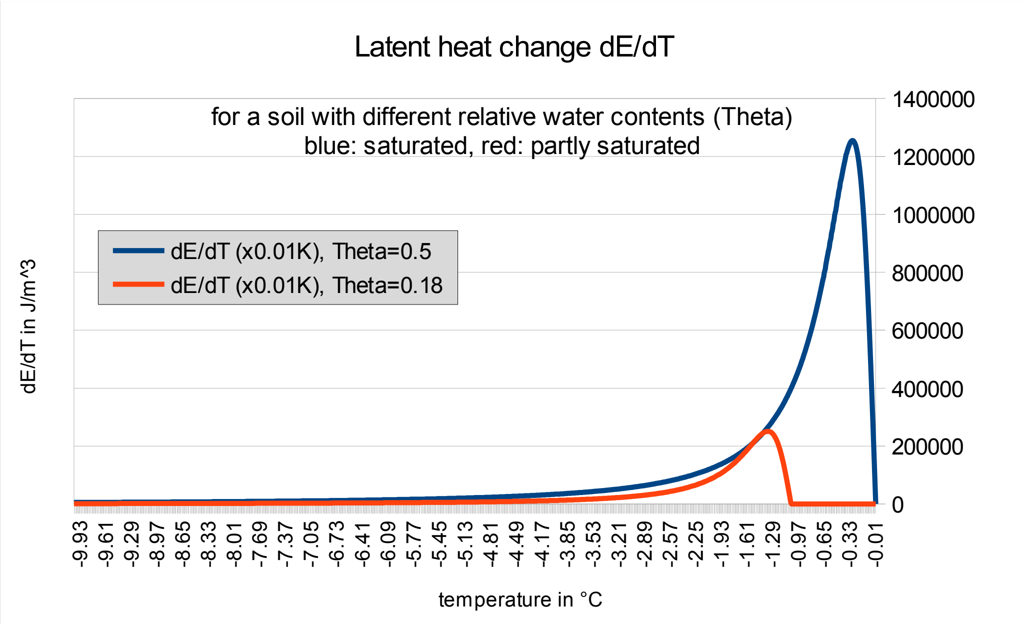

Figure 6: The change in energy, i.e. latent heat, per temperature change of 0.01°C for a soil with $\Theta_s = 0.5$ and $\Theta_r = 0.1$ for saturated (Theta=0.5) and unsaturated (Theta=0.18) conditions

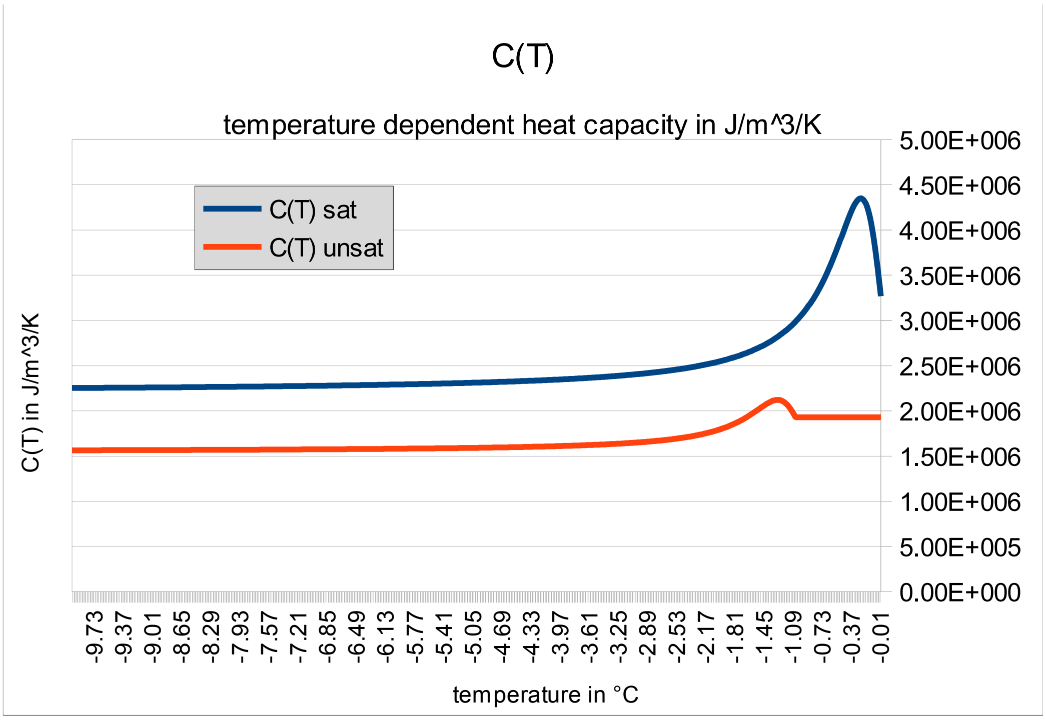

Figure 7: The change in effective heat capacity of a freezing/thawing soil (Θ_s = 0.43 and Θ_r = 0.06) for saturated (Theta=0.5) and unsaturated (Theta=0.18) conditions.

Estimation of the temperature shift for unsaturated soils

Figure 6 shows the energy change with temperature for a saturated soil (blue) and an unsaturated soil (red). The red curve is reduced according to the relative free water content (liquid or frozen) of the soil (which is 0.2 in this example) and shifted to lower temperatures in a way that there should be no higher energy changes for any temperatures than for the same temperature in an saturated soil. This constraint is a result of considering the physics of freezing soils. Since equation (2.24.10) is quite complex for an analytical solution of the derivative, the steps described below will be done numerically by using lookup-tables in the model to speed up the program. The aim is to shift the reduced curves for unsaturated soils in a way that the maximum of the reduced energy change curve comes as near to the left branch of dE/dT as possible without letting the reduced energy change curve cross the saturated energy change curve (slight overshooting is allowed to simplify the shifting procedure).

Step 1: Finding the maximum energy change $\max(dE/dT)_{sat}$ and the corresponding temperature $T_{\max dE,sat}$ for saturated soils. This could be done by setting the first derivative, which is the second derivative of E itself, to zero and solving for T. Since this is analytically not feasible (the resulting equation is some rows long...), it is done by numerical interpolation between the values of a lookup table containing the derivatives of dE/dT.

Step 2: Calculating the reduced maximum for unsaturated soils which is $\max(dE/dT)_{sat} \cdot \Theta_{rel}$.

Step 3: Calculating the corresponding temperature for that energy change for saturated soils $T_{maxdE,unsat}$.

Step 4: The difference between the corresponding temperatures for the maximum energy change for unsaturated soil and the energy change in saturated soils corresponding to the maximum for unsaturated soil $T_{\max dE,sat} - T_{maxdE,unsat}$ is the basic temperature shift.

Step 5: The maximum of the reduced curve should be shifted a little bit to the right of the point calculated in steps two and three, so an empirically found correction factor of $f_c = 1.15$ (a range of 1.1...1.2 seems to be possible depending on main soil type, but 1.15 works good for a wide range of soils) is applied to the temperature shift from step four since this was computed as temperature difference between the peaks of saturated and unsaturated energy change, but we want the reduced curve to meet the unsaturated curve as asymptotically as possible at the left decreasing branche.

The effective temperature as used in equations (2.24.6) and (2.24.10) can such be expressed by

$$T_{eff} = T - \left(T_{max(dE/dT),unsat} - T_{max(dE/dT),sat} \cdot f_c \right) \qquad \textbf{(2.24.10a)}$$

in order to reduce the additional shift by factor f_c for saturation values near full saturation, factor f_c is reduced linearly to zero as soon as the temperature difference for the maxima of saturated and unsaturated soils get smaller than the double offset:

$$\begin{aligned} f_c &= 1.15 \quad \text{for} \quad T_{max(dE/dT),unsat} < T_{max(dE/dT),sat} \cdot (1 + 2 \cdot (f_c - 1)) \\ f_c &= 1 + 0.5 \cdot \frac{T_{Max(dE/dT),unsat} - T_{max(dE/dT),sat}}{T_{max(dE/dT),sat}} \quad \text{for all higher} \quad T_{max(dE/dT),unsat} \end{aligned} \qquad \textbf{(2.24.10b)}$$

If the water content arrives saturation, f_c is going to 1.0, so the temperature shift is zero at this pont as should be epected.

Modeling the temperature change

At this point, the above equations (2.24.6) to (2.24.10) can be used to calculate temperature changes in a given soil volume. Equation (2.24.5) is repeated here for clarity:

$$\rho \cdot V \cdot C(T) \cdot \frac{\Delta T}{\Delta t} = \lambda(T) \cdot \frac{A}{L} \cdot \Delta T = Q_{in} - Q_{out} + q_s \qquad \textbf{(2.24.11)}$$

Eq. 2.24.11 (or Eq. 2.24.5) is the discrete form of Eq. (2.24.3). The heat transfer model (conduction and advection) described here for the WaSiM soil model is 1D vertical only. The model domain is presented in figure 8.

The layer of interest is the layer with index i. The layer above is layer i-1, the layer below is layer i+1. Q_{in} in equation (2.24.11) is the heat flow from layer i-1 to layer i (upper arrow), Q_{out} is the heat flow from layer i to layer i+1 (lower arrow). Each numerical layer may have its specific thickness d, but the effective length for heat transfer is calculated from center to center: for Q_{in}, the effective length is L_{i-1}, the effective length for Q_{out} is consequently L_{i+1}.
For clarity, the following heat flux equation refers to an elementary area A_e of 1m^2.

All variables of the left side of equation (2.24.11) can have specific values for each layer (ρ will usually be identical, but V and $C(T)$ may change). Parameters like λ, C, S_E and others will have to be averaged based upon the properties of both involved layers that represent the domain for fluxes Q_{in} and Q_{out}.

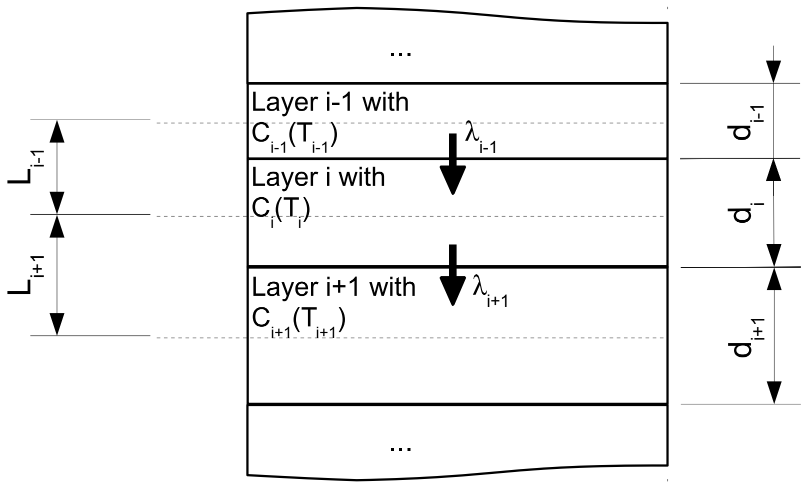

Figure 8: Definition of layer indices for the discrete 1D heat transfer model describing heat transfer through conduction.

Having defined the model domain for the discrete heat flux model, the fluxes Q_{in} and Q_{out} can be written as:

$$Q_{in} = \lambda_{i-1}(T_{i-1}) \cdot \frac{A_e}{L_{i-1}} \cdot (T_{i-1} - T_i) \qquad [\mathrm{J \cdot s^{-1}}] \qquad \textbf{(2.24.12)}$$

and

$$Q_{out} = \lambda_{i+1}(T_{i+1}) \cdot \frac{A_e}{L_{i+1}} \cdot (T_i - T_{i+1}) \qquad [\mathrm{J \cdot s^{-1}}] \qquad \textbf{(2.24.13)}$$

Note that the values of $\lambda_{i-1}(T_{i-1})$ and $\lambda_{i+1}(T_{i+1})$ are **not** the values valid for their respective layers but effective values for the distance or volume between the centers of the involved layers.

The equation for the temperature change is achieved by using (2.24.12) and (2.24.13) for the respective terms in (2.24.11) and isolating ΔT on the left side:

$$\Delta T_i = \frac{\Delta t}{\rho \cdot V \cdot C(T_i)} \cdot \left[\lambda_{i-1}(T_{i-1}) \cdot \frac{A_e}{L_{i-1}} \cdot (T_{i-1} - T_i) - \lambda_{i+1}(T_{i+1}) \cdot \frac{A_e}{L_{i+1}} \cdot (T_i - T_{i+1}) + q_s \right] \qquad \textbf{(2.24.14)}$$

Eq. (2.24.14) allows a calculation of the change in temperature for each numerical soil layer (since this is an explicit solution which is supported in WaSiM for conduction only, the term q_s is not regarded specifically here; the implicit solution schema however is using additional sources and sinks, see below).

Boundary conditions:

The finite difference scheme needs to have an upper and a lower boundary condition. The **upper boundary condition** will be the air temperature modified by an n-factor (Kade et al. 2006) as no physically based heat transfer modelling of snow cover is yet implemented in WaSiM. The n-factor, the ratio of seasonal thawing or freezing degree-day sums at the soil surface to that in the air, integrates the effects of all surface factors of the soil thermal regime and is the ratio of soil surface temperature to air temperature. In WaSiM, the n-factor can be defined in the control file with mean monthly values. .. A factor of 1 means that the air temperature is taken without scaling as upper boundary condition. Lower n-factors will lead to colder soil surface than air temperature in summer and warmer soil surface temperatures than air temperatures in winter.

There are two methods to define the lower boundary condition: A constant temperature or a constant heat flux. The latter is recommended for long-term simulations (>10 yrs).
The constant temperature condition can be defined either globally or as a grid value for each cell.

1) Global definition (is used if no grid with identifier "`T_Lower_Boundary_Condition`" is found): The default value for the mean annual temperature, normalized to sea level is defined together with a temperature lapse rate (e.g. -0.7 K/100m). These values are then used to estimate the temperature at the lower soil boundary. For example, a meteorological station in the watershed is located at 350 m elevation and has a mean annual air temperature of 5.55 °C. Here, the normalized sea level air temperature would be 8 °C (calculated from 5.55+3.5*0.7). This would of course result in a lower boundary condition at the meteorological station of 5.55°C (8-3.5*0.7). Accordingly, at another location in the watershed, let's say with a ground surface elevation of 700 m, the lower boundary condition would be 0.65°C (from 5.55-7*0.7). This scheme is applied at start-up for each cell.
2) As a pre-defined Grid: An additional standard grid will be read in, containing the temperature at the bottom of the soil column (e.g. 5.55 for the given grid cell from the example above). The grid must be assigned the internal identifier "`T_Lower_Boundary_Condition`" in the control file. A pre-defined grid allow the user to custom design the lower boundary conditions based on for example, differences in air temperature and variables affecting local n-factors, which can dramatically modify mean annual soil surface temperatures (and therefore the lower boundary condition).

If the **lower boundary condition** should be defined as a **constant heat flux**, an *additional* boundary condition grid needs to be identified as "`HeatFlux_Lower_Boundary_Condition`". The constant heat flux is applied by calculating the resulting temperature difference between the lower boundary and the lowest numerical layer for the given heat flux. The resulting temperature is then set as lower boundary condition value ("constant" temperature) for every time step. Note that an T_Lower_Boundary_Condition–grid is still needed for this method for initialization purposes (see below). The measure of the grid cells for the constant heat flux is in W/m^2. Typical values are $65 mW/m^2$ (world-wide average), so the value in the grid should be around 0.065. There exist some maps for the geothermal gradient (which is often expressed in W/m^2). Values range from $<40 mW/m^2$ to around $1 W/m^2$ and more, especially in geologically active regions.

Initial values of soil temperatures conditions:

The most basic initialization of the soil temperature profile in WaSiM assumes a linear gradient between the lower boundary condition and the upper boundary condition (air temperature modified by the n-factor) as provided by the forcing data that is informing the first model time step. This means, that the user still has to define the lower boundary temperature via the `T_Lower_Boundary_Condition`-grid even if the constant heat flux method has been chosen. Note that the `T_Lower_Boundary_Condition`-grid or the default global boundary temperature settings are only used at the very first model time step if the boundary condition method is set to use the constant heat flux (i.e. if a `HeatFlux_Lower_Boundary_Condition-grid` is found). This implies that the initial conditions strongly depend on the model start date, since the upper boundary conditions (air temperature and n-factor) experiences seasonality.

When starting WaSiM with initialization from formerly stored grids, the temperatures are read in as a grid-stack (like soil water content etc.) and the model run can start with the correct (modeled) soil temperatures (no initializing from the boundary conditions occurs).

How does the numerical scheme work?

For the numeric solution, the various calculation steps are arranged as follows:

1. computing the length of the sub time step for the heat transfer model (by using the so called mesh Fourier number when using an explicit solution scheme or by the manually defined sub time step limits) and the sub time step for the Richards solution scheme (heat transfer sub time step will always be smaller or equal to the Richards sub time step)
2. start of a sub time step
3. estimating the relative (water to ice) saturation S_E
4. estimating the hydraulic conductivity using the van-Genuchten parameters and Eq. (2.24.8c) from the actual water saturation, Θ_{act} and the actual relative Saturations, S_E and S_R.
5. estimating the effective thermal conductivities
6. estimating the effective heat capacities
7. calculating the heat fluxes, the temperature differences and finally the resulting new temperatures using either explicit or implicit solution schemes (when using implicit schemes, only the new temperatures are calculated directly)
8. checking for breaks of the second law of thermodynamics (i.e. no source region may cool down to temperatures below the temperature of the target region) – restrict the fluxes if necessary or set a smaller time step. This is a security measure against numerical instabilities when using the explicit solution method
9. repeat heat transfer computation if necessary (depending on the ratio of the sub time step for heat transfer and the sub time step for soil water balance) --> go to step 3
10. calculating mass fluxes using the Richards approach
11. run the next sub time step for soil water balance

Note: Since the heat transfer is not limited to the unsaturated zone of the soil, the model domain of the Richards-Equation and the model domain of the heat transfer equation will differ: The Richards-approach is only applied to the unsaturated (numeric) soil layers, whereas the heat transfer must be calculated for each layer down to the lower boundary condition, i.e. for the entire soil column. In order to keep the computation speed as fast as possible, both algorithms will be processed separately but in the same main iteration loop (for sub time steps of the soil water balance): Each equation is applied to the respective model domain before calling the other equation or the next sub time step.

Some additional features were implemented into the model to optimize the performance. These are mainly a sub time step optimizer, and a scheme preventing the heat transfer model from inverting gradients when the sub time step was chosen too long (for explicit solution schemes):

1) Optimizing sub time steps: Even when WaSiM runs in hourly time steps, the duration of an interval is much too long to realistically calculate the heat flow into or between thin soil layers. So the internal time step has to be set to much smaller values down to a few seconds (depending on several parameters like layer thickness, soil water content, freezing state and temperature gradient and van-Genuchten parameters). On the other hand, if the temperature gradients are small, the time step can be as large as some minutes. Since this is quite critical in terms of model performance, an internal sub time step optimizer was implemented. The optimal sub time step for heat transfer may be shorter or longer than the optimal time step for the Richards approach (which is estimated by evaluating the Courant-condition). The minimum of both sub time steps will be the winner, so the model will satisfy the heat transfer as well as the water transport. The following algorithm is applied to each soil layer, to each cell, and in each time step to get the optimal sub time step:
   1. running the complete scheme down to point 6 (see above description of the numeric scheme)
   2. computing the so called mesh Fourier number F_M which must be less than 0.5 in order to prevent the solution from oscillating and getting the maximum time step by:

$$F_M = \frac{\lambda \cdot \Delta t}{(\Delta x)^2} \quad \rightarrow \quad with\, F_M \leq 0.5 \quad \rightarrow \quad \Delta t \leq \frac{0.5 \cdot (\Delta x)^2}{\lambda} \qquad \textbf{(2.24.15)}$$

   3. The split factor (as quotient of the nominal time step and the *Δt* from the above equation) can be limited by model parameters: the minimum sub time step and the maximum sub time step can be set manually. So the computed optimal split factor can be limited in both directions in order to prevent numeric instabilities. It is recommended to make some tests using the test data set and playing with the soil parameters and other input (rain etc.). The recommended values are between 3 seconds for the minimum sub time step and around 60 to 180 second for the maximum sub time step for the explicit solution, depending on layer thickness and hydraulic parameters. When using the implicit solution, the minimum sub time step may also be much longer, since the approach is more stable (up to 1800 seconds or even more → make tests!).
   4. This split-factor is then compared with the split-factor computed for the Richards approach. The larger value will be taken as effective split factor for the actual cell.

2) Limiting the heat transfer: If for some reason the sub time step was not sufficient to keep the model on safe ground (which means: no numerical instabilities), another backup algorithm is taking over. This may happen because the minimum or maximum allowed sub time step was set wrongly or because the gradients are beyond the assumptions (only top to bottom gradients were checked). There are four checks executed for each numeric soil layer:

   1. if the heat is flowing upwards through the layer (see equations 2.24.12 and 2.24.13 and figure 8 for reference):

$$\text{if}\,(Q_{in} \geq 0 \wedge Q_{out} \geq 0) \;\; \text{then} \;\; T_i \leq T_{i+1} \rightarrow \text{limit } T_i \text{ to } T_{i+1} \qquad \textbf{(2.24.16)}$$

   if the heat if flowing out to the upper as well as to the lower layer:

$$\text{if}\,(Q_{in} \geq 0 \wedge Q_{out} < 0) \;\; \text{then} \;\; T_i \geq min(T_{i+1}, T_{i-1}) \rightarrow \text{limit } T_i \text{ to } T_{i+1} \text{ or to } T_{i-1} \qquad \textbf{(2.24.17)}$$

   2. if the heat is flowing upwards through the layer

$$\text{if}\,(Q_{in} < 0 \wedge Q_{out} < 0) \;\; \text{then} \;\; T_i \leq T_{i-1} \rightarrow \text{limit } T_i \text{ to } T_{i-1} \qquad \textbf{(2.24.18)}$$

   3. If the heat is flowing into the layer from the upper layer as well as from the lower layer:

$$\text{if}\,(Q_{in} < 0 \wedge Q_{out} \geq 0) \;\; \text{then} \;\; T_i \leq max(T_{i+1}, T_{i-1}) \rightarrow \text{limit } T_i \text{ to } T_{i+1} \text{ or to } T_{i-1}$$

(2.24.19)

However, this mechanism cannot prevent the model completely from numeric instabilities, it can only prevent the model from "exploding". A better way to prevent numerical instabilities is to use the implicit time-stepping solution (backward Euler integration), which is briefly described in the following paragraphs.

Solution schemes

There are two possible solution schemes: the explicit and the implicit solution scheme.
The **explicit scheme** is also known as explicit time stepping or the forward Euler integration. It is straightforward and uses exactly the equations given above (but without advection!). The temperatures at time n+1 are depending solely on the temperatures at time n, so the solution can be directly taken from the solution of equation (2.24.14).

However, the explicit solution tends to be numerically unstable, especially if limiting the sub time step length to a given minimum. This means that a model with an explicit solution will need more time to run in a stable state. On the other hand, an **implicit solution** (also known as backward Euler integration or implicit time stepping) uses the (not known) temperatures at time n+1 to define the temperatures at any layer. This results in a linear system of equations which is shown here as an example:

Let's use eq. (2.24.11) with some modifications:

$$\Delta T_i = T_{i,n+1} - T_{i,n} = \frac{\Delta t}{x_i \cdot C_i} \cdot \left(Q_i - Q_{i-1}\right) - q_{i-1} \cdot c_w \left(T_{i,n} - T_{i-1,n+1}\right) - q_{i+1} \cdot c_w \left(T_{i+1,n+1} - T_{i,n}\right) - q_{mac} \cdot c_w \left(T_{mac} - T_{i,n}\right) \quad \textbf{(2.24.20)}$$

where
T is the temperature in layer i [°C]
i denotes the numerical layer index
n denotes the time index (n is actual time, n+1 is one sub time step later)
Δt is the sub time step (see eq. (15)) [s]
x is the layer thickness [m]
C is the actual heat capacity of that layer [J/(m^{3}K)]
Q is the actual heat flux between the layers (index i denotes flux between layer i+1 and i, index i-1 denotes flux between layer i-1 and I)
q_{i-1} is the water flux between the upper and the actual layer; upward is positive [m/s]
q_{i+1} is the water flux between the lower and the actual layer; upward is positive [m/s]
q_{mac} is the water flux from macropore infiltration (always >= 0) [m/s]
c_w is the specific heat capacity of liquid water [J/(m^{3}K)]
T_{mac} is the temperature of macropore infiltration water, which is set to either 0°C from snow melt or to the air temperature for infiltrating rain water [°C]

By using the individual thicknesses and thermal conductivities as well as actual heat capacities of each layer (remember: each numerical layer can have a distinct set of parameters), eq. (2.24.20) can be written as:

$$T_{i,n+1} - T_{i,n} = \frac{\Delta t}{x_i \cdot C_i} \cdot \left[\frac{\lambda_i}{-0.5 \cdot \left(x_i + x_{i+1}\right)} \cdot \left(T_{i,n+1} - T_{i+1,n+1}\right) - \frac{\lambda_{i-1}}{-0.5 \cdot \left(x_i + x_{i-1}\right)} \cdot \left(T_{i-1,n+1} - T_{i,n+1}\right) \right] - q_{i-1} \cdot c_w \left(T_{i,n} - T_{i-1,n+1}\right) - q_{i+1} \cdot c_w \left(T_{i+1,n+1} - T_{i,n}\right) - q_{mac} \cdot c_w \left(T_{mac} - T_{i,n}\right)$$

which, after isolating all factors for $T_{i-1,n+1}$, $T_{i,n+1}$ and $T_{i+1,n+1}$, resp., can be written as:

$$a_i \cdot T_{i-1,n+1} + b_i \cdot T_{i,n+1} + c_i \cdot T_{i+1,n+1} = T_{i,n} - \frac{\Delta t}{x_i \cdot C_i} \cdot q_{mac,i} \cdot c_w \cdot T_{mac} \qquad \textbf{(2.24.21)}$$

with

$$\begin{aligned} a_i &= -\frac{2 \cdot \Delta t \cdot \lambda_{i-1}}{x_i \left(x_i + x_{i-1} \right) \cdot C_i} - \frac{q_{i-1} \cdot c_w \cdot \Delta t}{x_i \cdot C_i} \\ c_i &= -\frac{2 \cdot \Delta t \cdot \lambda_i}{x_i \left(x_i + x_{i+1} \right) \cdot C_i} + \frac{q_{i+1} \cdot c_w \cdot \Delta t}{x_i \cdot C_i} \\ b_i &= 1 - a_i - c_i - \frac{q_{mac} \cdot c_w \cdot \Delta t}{x_i \cdot C_i} \end{aligned} \qquad \textbf{(2.24.22)}$$

Such a linear equation as given in eq. (2.24.21) can be formulated for each of the *m* numerical layers, resulting in *m* equations with *m*+2 unknowns. Since the upper and the lower boundary conditions as well as all terms on the right side of (2.24.21) are known, the number of unknowns is reduced to *m*, thus resulting in a set of *m* linear equations with *m* unknowns ($T_{i-1,n+1}$ for layer 1 is the known upper boundary condition, $T_{i+1,n+1}$ for the bottom layer is the lower boundary condition, the respective terms with their factors are moved to the right hand side). All the other known right hand values are the temperatures at time *n*. This set of equations can now be seen as a tri-diagonal or tri-banded matrix which has to be solved to get the temperatures at time *n*+1. The solution of such a tri-banded matrix is computational very effective (and is not described here, see e.g. Wikipedia for reference). Note that the equations (2.24.21) and (2.24.22) will turn into the pure heat conduction form when there is no advection, since all the additional terms will then be zero.

Note: Equations (2.24.21) and (2.24.22) look a bit different for the uppermost and lowermost layer, since

- the temperatures $T_{i-1,n+1}$ for the top layer and $T_{i+1,n+1}$ for the bottom layer are the known boundary conditions
- the distance between the center of the top and bottom layer to the respective boundary is only one half of the respective layers thicknesses
- factors a (for upper boundary condition) and c (for lower boundary conditions) are set to zero (in the tri-banded matrix' left hand side, not on the right hand side) in order to have a reasonable systems of equations.

Thus, the top layers equation looks like this:

$$\begin{aligned} b_1 \cdot T_{1,n+1} + c_1 \cdot T_{2,n+1} &= T_{1,n} - \frac{\Delta t}{x_1 \cdot C_1} \cdot q_{mac,1} \cdot c_w \cdot T_{mac} - a_1 \cdot T_{0,n+1} \\ &\text{with} \quad x_0 = 0 \text{ and } T_{0,n+1} = T_{air} \text{ for no snow and 0°C for snow:} \\ b_1 \cdot T_{1,n+1} + c_1 \cdot T_{2,n+1} &= T_{1,n} - \frac{\Delta t}{x_1 \cdot C_1} \cdot q_{mac,1} \cdot c_w \cdot T_{mac} + T_{air} \cdot n_f \cdot \left[\frac{2 \Delta t \cdot \lambda_1}{x_1^2 \cdot C_1} + \frac{q_0 \cdot c_w \cdot \Delta t}{x_1 \cdot C_1} \right] \end{aligned} \qquad \textbf{(2.24.23)}$$

where q_0 in the braced term is the infiltrating water and $T_{0,n+1}$ was replaced by applying the air temperatur T_{air} and the f-factor n_f.

Accordingly, the equation for the bottom layer can be written like this:

$$a_i \cdot T_{i,n+1} + b_i \cdot T_{i,n+1} = T_{i,n} - \frac{\Delta t}{x_i \cdot C_i} \cdot q_{mac,i} \cdot c_w \cdot T_{mac} + T_{low} \cdot \left[\frac{2 \Delta t \cdot \lambda_i}{x_i \cdot C_i \cdot (x_i + x_{i+1})} - \frac{q_{i+1} \cdot c_w \cdot \Delta t}{x_i \cdot C_i} \right]$$

$$\text{with } x_{i+1} = 0 \text{ and } q_{i+1} = 0: \qquad \textbf{(2.24.24)}$$

$$a_i \cdot T_{i,n+1} + b_i \cdot T_{i,n+1} = T_{i,n} - \frac{\Delta t}{x_i \cdot C_i} \cdot q_{mac,i} \cdot c_w \cdot T_{mac} + T_{low} \cdot \frac{2 \Delta t \cdot \lambda_i}{x_i^2 \cdot C_i}$$

If the lower boundary condition is a constant heat flux, which may not necessarily be constant for the entire model run but temporally variable by reading in a new standard grid every month or so for the “`HeatFlux_Lower_Boundary_Condition`”-grid, equation (2.24.24) can still be used, although the lower boundary condition is used as constant temperature there. The solution is simple: A constant heat flux can be defined like this:

$$q_{low} = \lambda_i \cdot \frac{\Delta T}{x_i \cdot 0.5} \qquad \textbf{(2.24.25)}$$

where q_{low} is the heat flux through the lower boundary into the bottom layer of the heat transfer and soil model in W/m^2 or J/(s·m^2); λ_i is the thermal conductivity of the bottom layer in W/(m·K) or J/(s·m·K); x_i is the layer thickness of the bottom layer (and 0.5 is a factor to account for the fact that the flux is calculated between the lower boundary and the center of the bottom layer only). To get an estimation for the lower boundary temperature that creates this flux, the term ΔT is split into $T_{low} - T_i$ and then T_{low} is isolated:

$$T_{low} = T_{i,n} + \frac{x_i \cdot q_{low}}{2 \cdot \lambda_i} \qquad \textbf{(2.24.26)}$$

So if a constant heat flux is used instead of a constant temperature method, equation (2.24.26) replaces T_{low} in equation (2.24.24) before solving the equation system.

The big advantage of such an implicit solution is the numerical stability. This allows for longer sub time steps to be used. However, one should be careful to set the sub time step not to a too large value, since the specific heat capacity can be, depending on the van-Genuchten parameters) quite sensitive to temperature changes, resulting in incorrect temperatures when using too long time steps. The disadvantage of the implicit solution is the in-accurateness when the time steps get too long (which risk can of course be minimized by choosing shorter minimal sub time steps).

A series of tests resulted in the recommendation that for daily time step the sub time step for explicit solutions should not be larger than 1800 seconds, whereas for implicit solutions, the time step can still be as large as a day without any substantial loss of accuracy. For hourly resolution, the situation is similar: explicit solution should not use larger time steps than 1200 s whereas for implicit solutions 3600 s are still useful. However, some artificial effects will be seen in both versions because of the larger temporal temperature gradients within a day, so shorter time steps are recommended as down to 900s for both methods when running in an hourly time step. Shorter input data resolution as well as thin numerical layers may require even shorter sub time steps.

Some Examples

Basics for applying the heat transfer model

For testing the heat transfer model and investigating the effects of different parameters on soil temperatures, a test data set is available from the author. The following examples are created using this test data set.

The test “basin” is a 10 x 10 cell area, 100 m cell size, 1 to 5 m elevation. The cell at row 5 and column 5 is the control plot.

The basin was set so that at almost every time step, all soil layers are saturated: cold climate, small evaporation amounts, regular precipitation (0.25mm per day), so there is no chance for drying out. Air temperature was represented by a sine-function of +/- 15°C annual amplitude for daily values, overlaid by a sine function with +/- 10°C for hourly values (so the temperatures vary between -25°C and -5°C at the end of December and between +5°C and +25°C at the end of June for hourly values). The input air temperatures are shown in figure 9 and figure 11. The tests were done with hourly and daily resolution.

The soil has 3 horizons with a 20cm organic top layer (10 layers of 2 cm each). Below that top horizon, 10 layers of 0.05 cm each form the second horizon representing mineral soil (50 cm thick) where the hydraulic conductivity is lower and the porosity is only 0.4. Below that, the third horizon reaches down to approx. 8.8 m depth through 81 layers of 10 cm each, where the lower boundary condition is defined as -10°C. The van-Genuchten parameters are identical for all layers in order to isolate the effect of heat transfer from other effects. Only the porosity of the upper horizon is set to high values as they are typical for boreal forest and arctic tundra.

Here is a ample of the soil parameterization in the soil table:

```
horizon                    = 1       2      3
DryHeatCapacity            = 810      800       900    ; # optional
parameters
DryDensity          = 450       900       1450   ; # optional parameters
DryThermalConduct   = 0.3       0.5       0.57   ; # optional parameters
Name                       = Peat    SIC    SIC         ;
ksat                       = 1e-4    1e-5   1e-7        ;
k_recession                = 0.9     0.9    0.9  ;
theta_sat                  = 0.8     0.40   0.30 ;
theta_res                  = 0.05    0.07   0.07 ;
alpha                      = 1.5     1.5    1.5  ;
Par_n                      = 2        2      2   ;
Par_tau                    = 0.5     0.5    0.5  ;
thickness                  = 0.02    0.05   0.1  ;
layers                     = 10      10     81   ;
```

The air temperature is taken as upper boundary condition with an n-factor of 1.0 (no damping or amplifying). No snow model was activated in order to demonstrate the effects of the soil heat transfer model only. A more practical example follows in figures ....

The result of the heat transfer model is shown in figures 10 and 12. Several interesting effects can be observed:

- damping of amplitude: the deeper the soil layer, the smaller the amplitude of the temperature changes
- time-shift of amplitude: the deeper the soil layer, the later the minimum and maximum occur
- larger temperature amplitudes for frozen soils compared to thawed soils (e.g. The red line in figure 10)
- no diurnal fluctuations below 50 cm (thawed) and 80-90 cm (frozen) resp.
- Almost no diurnal fluctuations during phase change
- phase change takes a long time (much energy must be transported into the soil to supply the latent heat for melting. Vice versa, during freezing, a lot of energy is set free, delaying the

freezing of the soil for a considerable amount of time

- the last effect in conjunction with the time shift leads to the situation that almost the entire thawed soil starts to freeze in late September / early October.
- The "wavy" shape of the temperature graphs is a numerical effect of the discretization. The temperatures are valid for the entire soil layer. So if a layer is thawing, the entire layer absorbs the latent heat for melting, thus affecting heat transfer to and from the lower and upper layer.

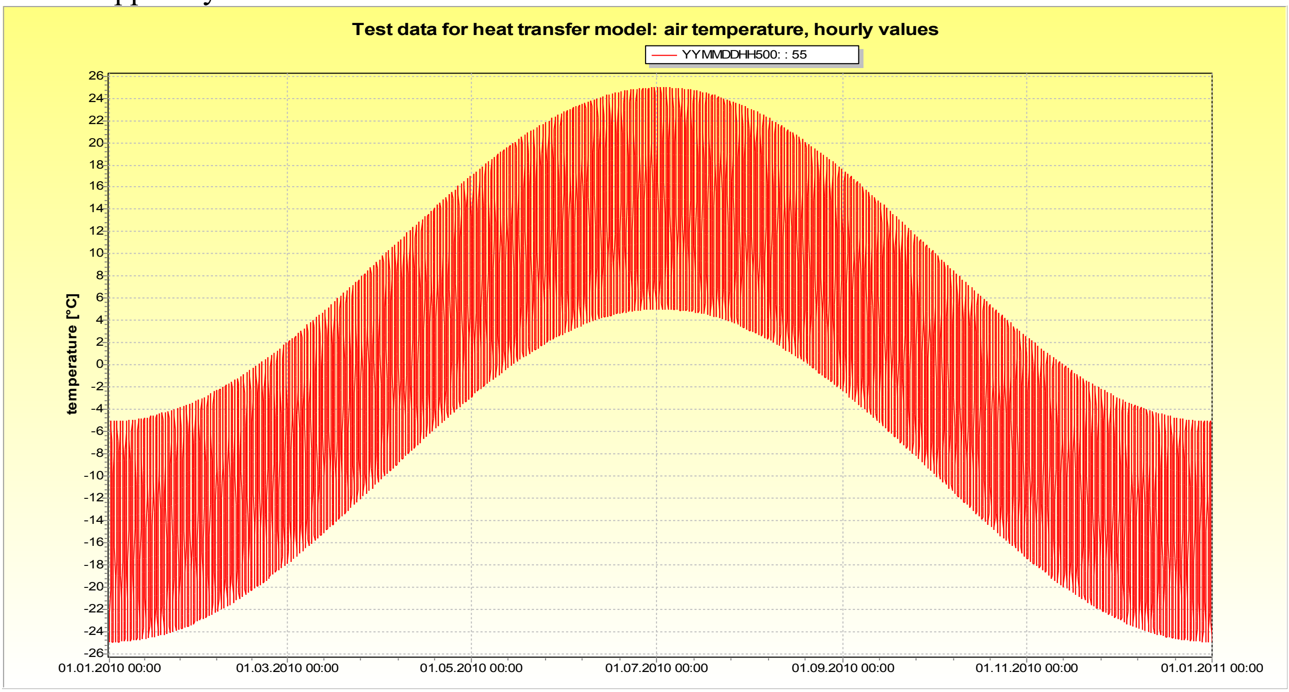

figure 9: temperatures used for heat transfer test data for hourly data (daily fluctuation +/- 10°C)

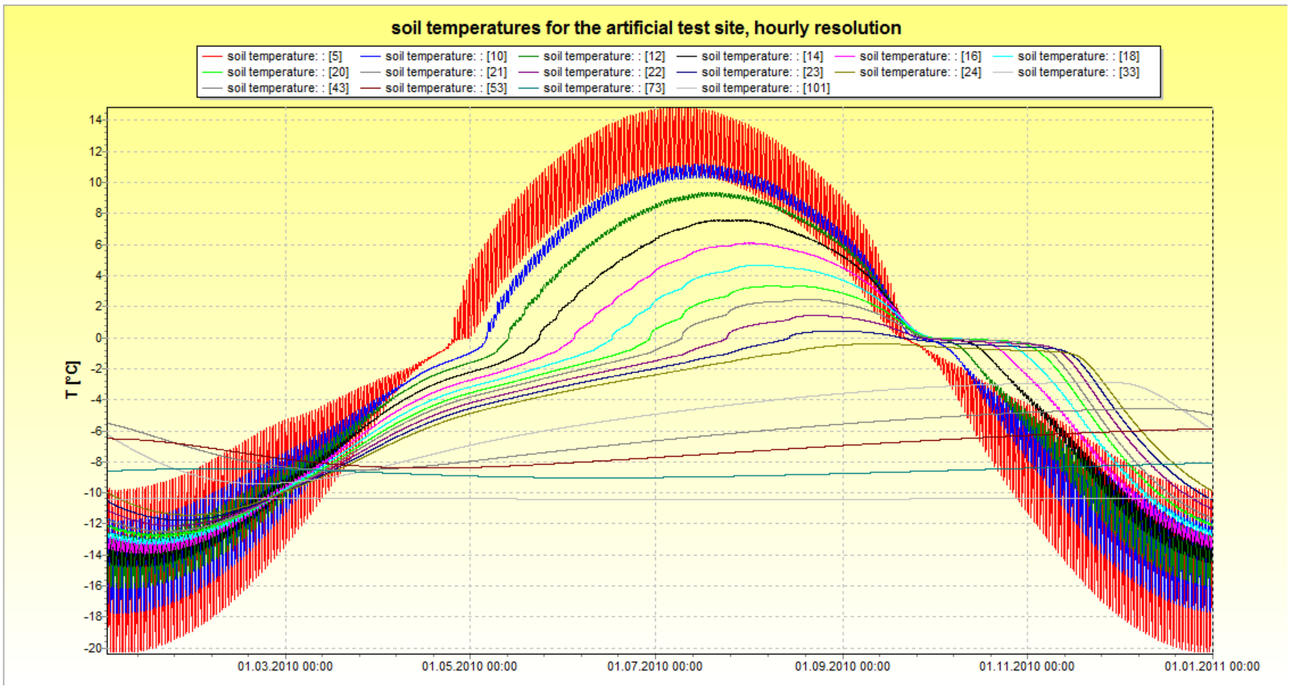

figure 10: soil temperatures for the artificial test site in hourly reslution (shown are temperatures for 10 cm to 110 cm in 10 cm steps and temperatures in 2, 3, 4, 7 and 8.8m)

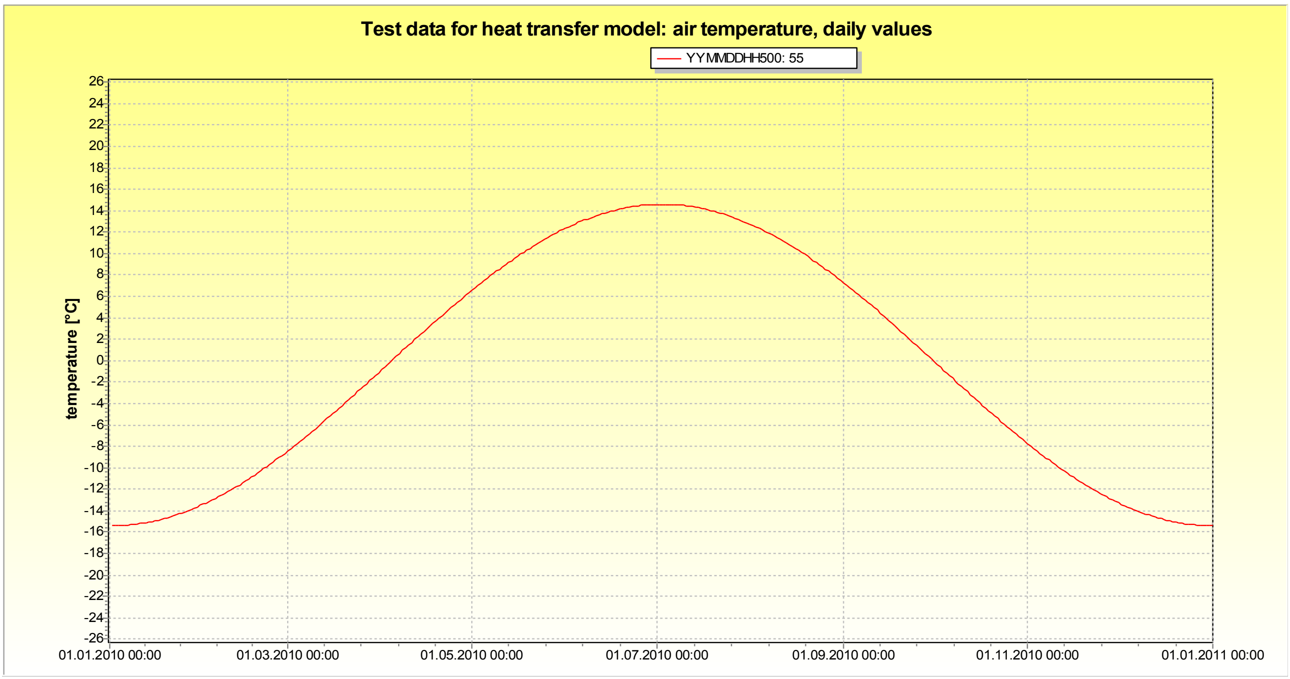

figure 11: temperatures used for heat transfer test data for daily data

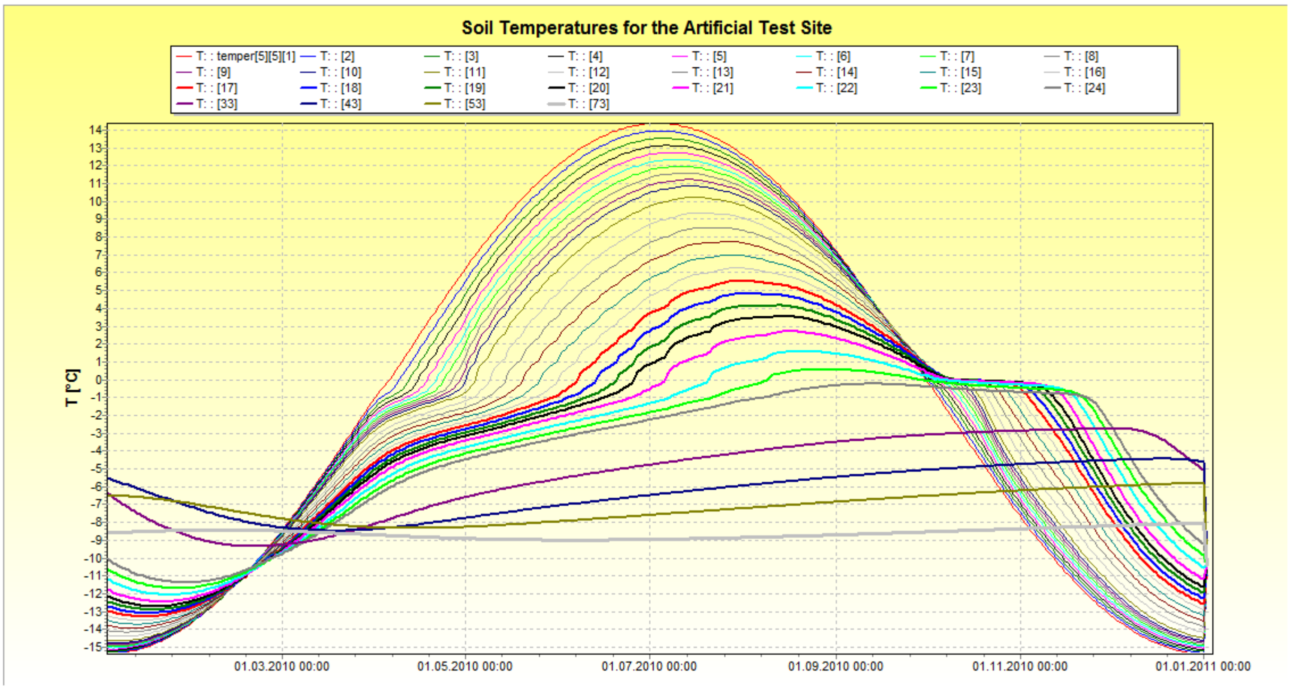

figure 12: soil temperatures for the artificial test site (upper horizon: 20 cm of organic material, modelled in 10 layers of 2 cm each, then 10 cm layers follow; profile has a total depth of 10 m --> the fat, dark grey graph is at around 7 m)

Figure 13 shows the active layer thawing and freezing as a sub-basin average. The results differ slightly: For hourly time steps, the thawing of deeper layers starts later, does consequently not reach as deep and the soils refreezes earlier. The physical background is simple: when the soil refreezes every night for a few weeks, the soil can transport more heat to the surface than it can transport from the surface into the soil at higher temperatures during the day: This is because the thermal conductivity of ice is much higher than for water. The algorithm to compute the thaw depth uses a parameter $SE_{threshold}$ which is the SE-value which should be treated as threshold for thawing/freezing. If this parameter is set to $SE_{threshold}$=0.8, the depth where SE (see eq. (6)) is at most 80% (i.e. $SE \leq 0.8$) is assumed to be the thaw depth.

Note: For some soil types (like loam and clay) the thaw depth will vary considerably from the thaw depth one would expect when measuring with e.g. a metal pole, especially when setting *TSE* to lower values like 0.5. Fig. 13 Shows the gray line as an example for hourly resolution with $SE_{threshold}$ = 0.8.

Note 2: The plotting program used to create figure 13 (Graphlines) cannot keep track of multiple freezing fronts so it looks like the entire soil column freezes at once, which is an artifact of the plotting software. The results from WaSiM shows freezing occurring both from the ground surface and from the permafrost table in early fall.

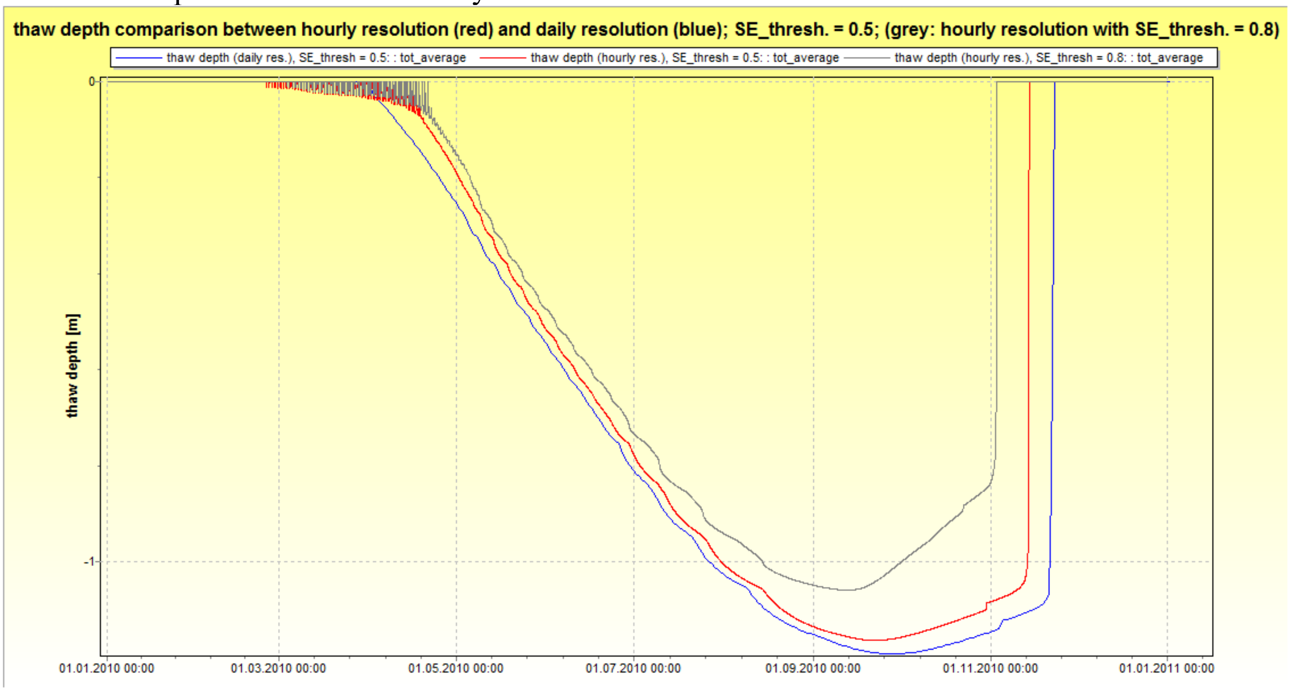

figure 13: Thaw depth for simulation in hourly and daily resolutions (red: hourly resolution with $SE_{threshold}$ = 0.5; blue: daily resolution with $SE_{threshold}$ = 0.5; grey: hourly resolution with $SE_{threshold}$ = 0.8)

Another, more realistic example is shown on the following figures 14 and 15. Here, real precipitation and temperature data for Barrow, Alaska, for 2007 was used (but printed as 2010 – never mind...). After snow melt in early June (which is not met exactly, it doesn't matter as well), the generated runoff was simply averaged here for demonstration purposes.

The runoff in figure 14 was generated without heat transport model. The soil is completely thawed, so the interflow component is large compared to figure 15, where the soil was frozen for most of the time (active layer was simulated to approx. 15 cm). The model didn't use the surface routing scheme, so the effects of the shallow melt water ponds cannot be modelled here, probably the evaporation is also not modelled correctly. But that is not the point. The point is, that the frozen soil leads to completely different runoff components and also to a different distribution over time.

One comment on model performance: when using very thin soil layers like 1 or 2 cm, the sub time step must be set to very small values (down to 3 seconds). Combined with large hydraulic conductivities and high porosities for the organic layer this may lead to very long computational times. It is therefore recommended, to use soil layers of e.g. 5 cm for the upper layer and then

10 cm or more for all other layers. If possible, the hydraulic properties of the uppermost layer should be set not to extreme values (not too high alpha and n values), in order to keep the sub time step as large as possible for the solution of the Richards equation. A run time factor of 2 to 10 with heat model compared to a model run without heat model can be expected even with such settings.

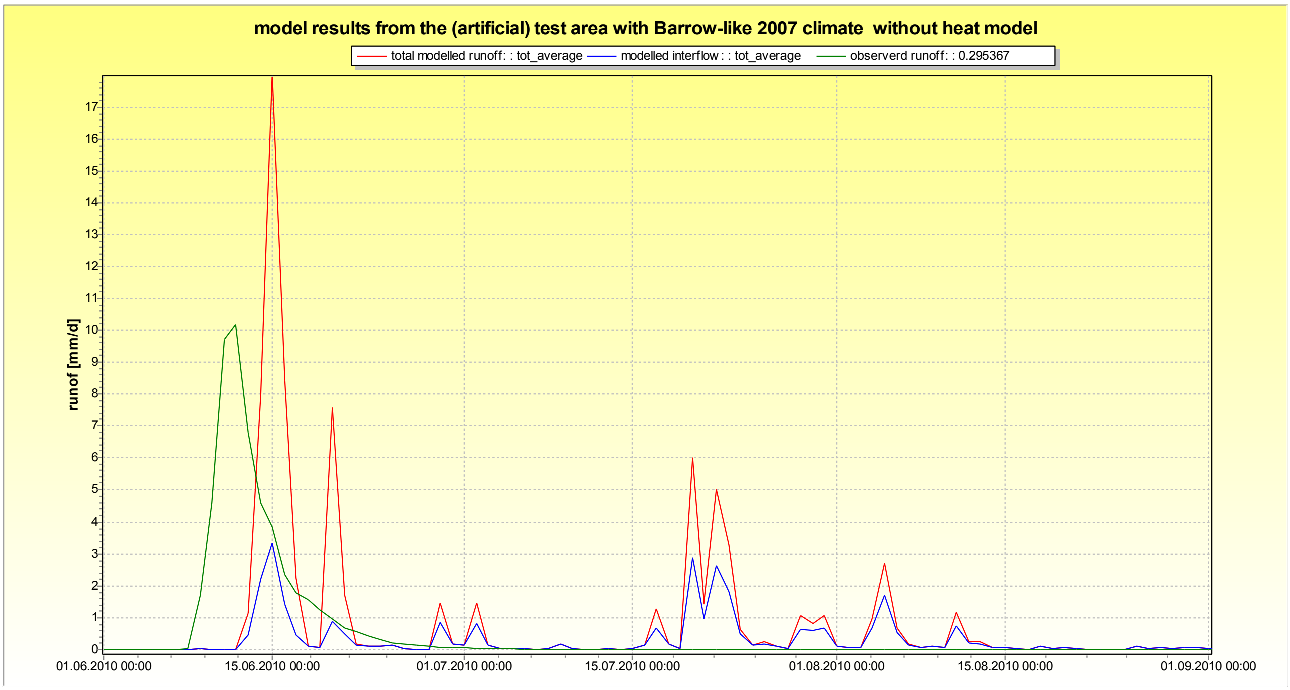

Figure 14: Model results from an artificial arctic test site with a Barrow-like climate without the soil heat transfer model. The curves represent observed runoff (green), total modeled runoff (red), and modeled interflow (blue).

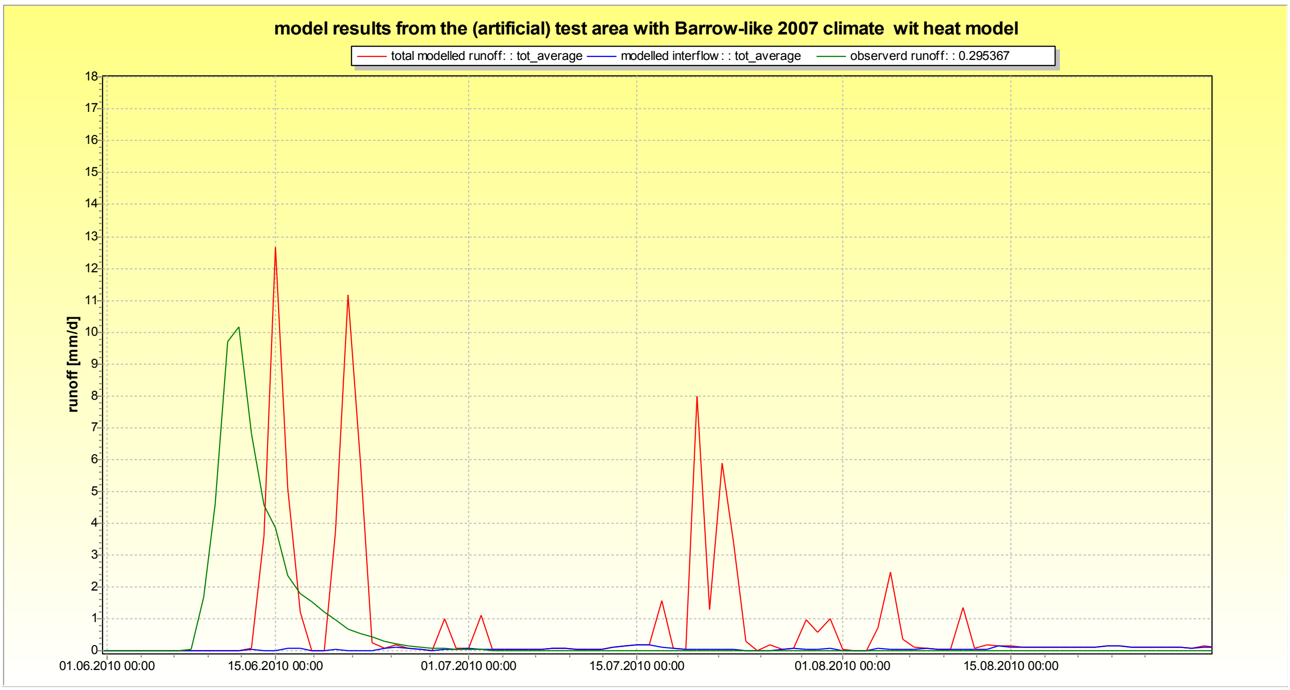

Figure 15: Model results from an artificial arctic test site with a Barrow-like climate with the soil heat transfer model. The curves represent observed runoff (green), total modeled runoff (red) and modeled interflow(blue).

Heat transfer example for different lower boundary conditions

Figure 16 shows the input to the next numeric experiment. It should show the difference between fixed temperatures and a constant heat flux as lower boundary conditions.

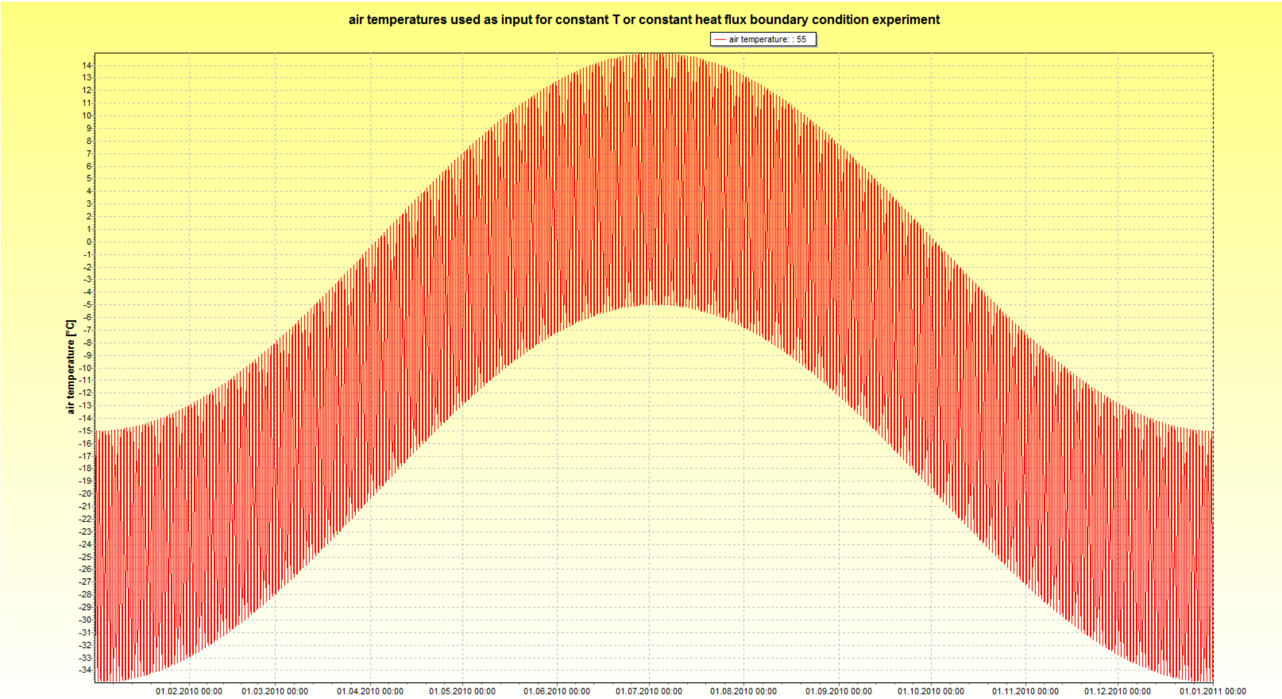

Figure 16: air temperature for the following experiments. T ranges from -25°C in winter to +5°C in summer with diurnal fluctuations of +/- 10°C. Annual average is -10°C

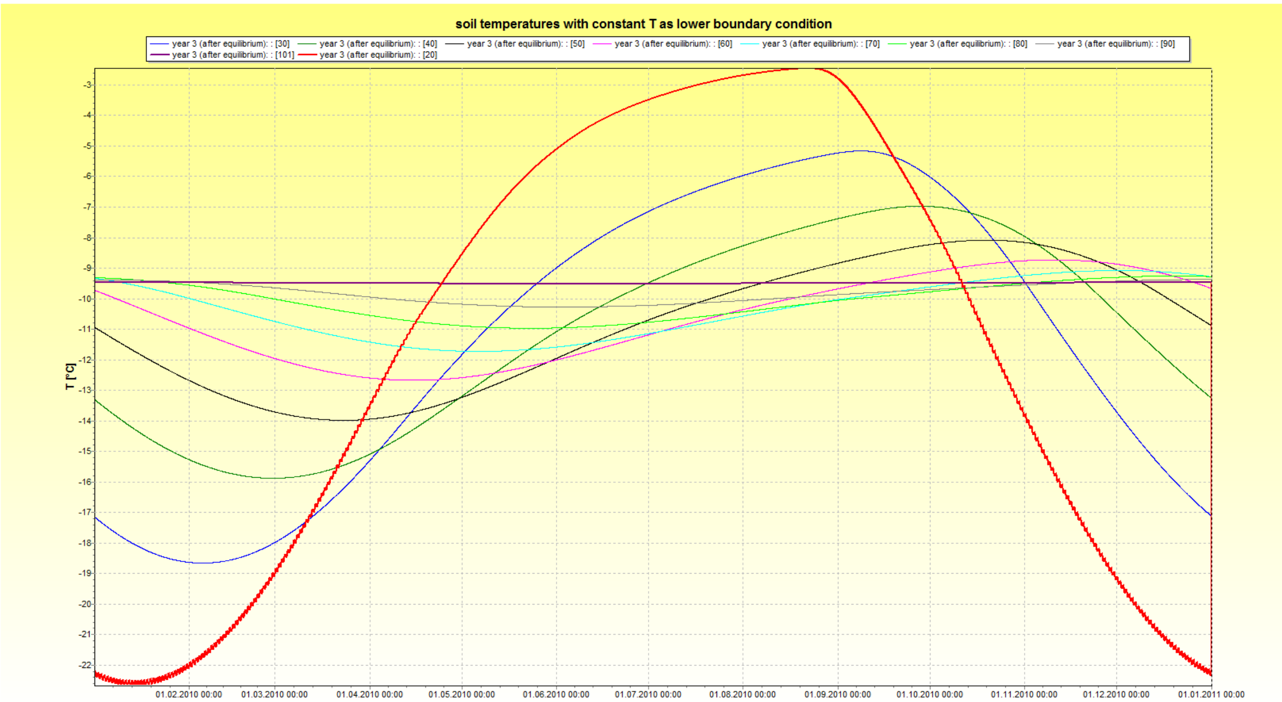

Figure 17: soil temperatures as time series for constant T lower boundary condition (red=0.7m, blue = 1.7m, green = 2.7m, black = 3.7m etc. down to 8.8m for violet)

As can be seen in figure 17 the lower boundary has a constant temperature of approx. -9.5°C. When changing the lower boundayry condition to a constant heat flux, that pattern changes, as can be seen in figure 18. Due to the deep temperatures of the entire soil, the temperatures at the lower boundary are even decreasing, despite the constant heat flux of 65 mW/m^2.

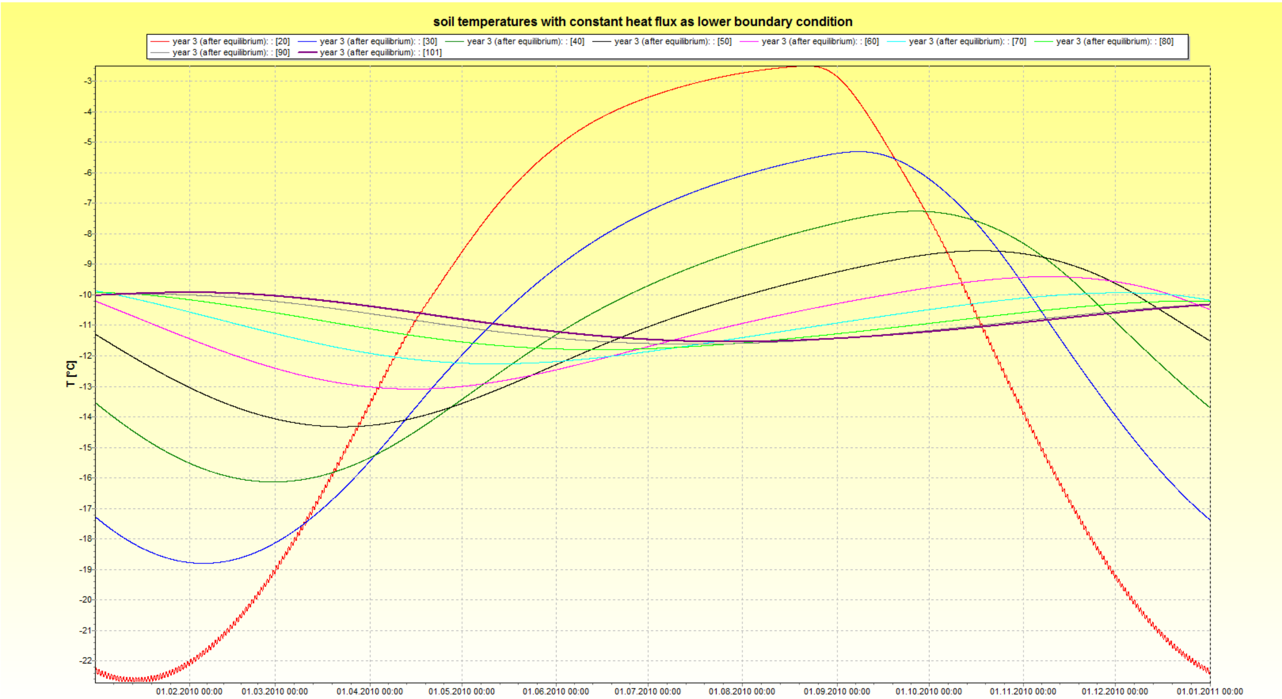

Figure 18: soil temperatures as time series for constant heat flux of 65mW/m^2 lower boundary condition (red=0.7m, blue = 1.7m, green = 2.7m, black = 3.7m etc. down to 8.8m for violet)

Another interesting comparison is shown in figures 19 and 20. Figure 19 shows the temperature profiles for four days in the hypothetical year 2010: January 1st, April 2nd, July 4th, and October 3rd (the choice of the four days has nothing to do with the national holidays of Slovakia (1/1), Iran (4/1), USA (7/4) and Germany (10/3) but with the minimum, maximum and inflection points of the temperature input ;-). For each of these days, the profiles for hours 1 and 13 are shown. The heat waves traveling through the soil can be clearly recognized: down to 50cm there is the diurnal variation due to the day/night changes of the surface temperature. Below that, the seasonal changes are visible. There is no significant change of temperature below ~9m. The October and April profiles are meeting at the uppermost layer – but they differ considerably in deeper layers, without any symmetry. At around -7m, the maximum temperature can be observed in winter and the minimum temperature in summer.

Figure 20 shows the same scenario with a constant heat flux of 65mW/m^2 as lower boundary condition. The overall temperatures are a little cooler, since 65mW/m^2 is not enough to compensate for the heat loss in winter (which is bigger than the heat gain in summer due to the higher heat conductivity of ice compared to water – in this experiment, no snow is taken into account and the n-factors are always 1.0).

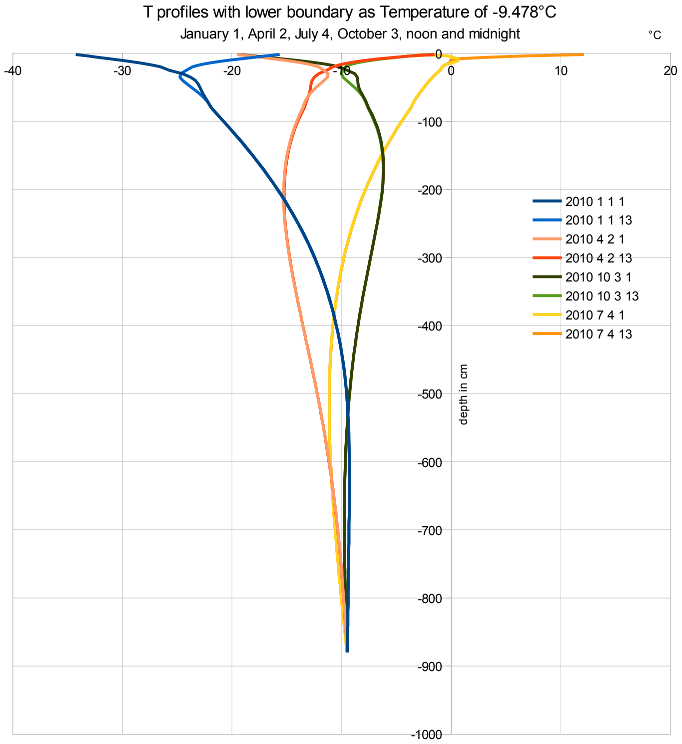

Figure 19: T-Profile with constant T -9.478°C as lower boundary condition

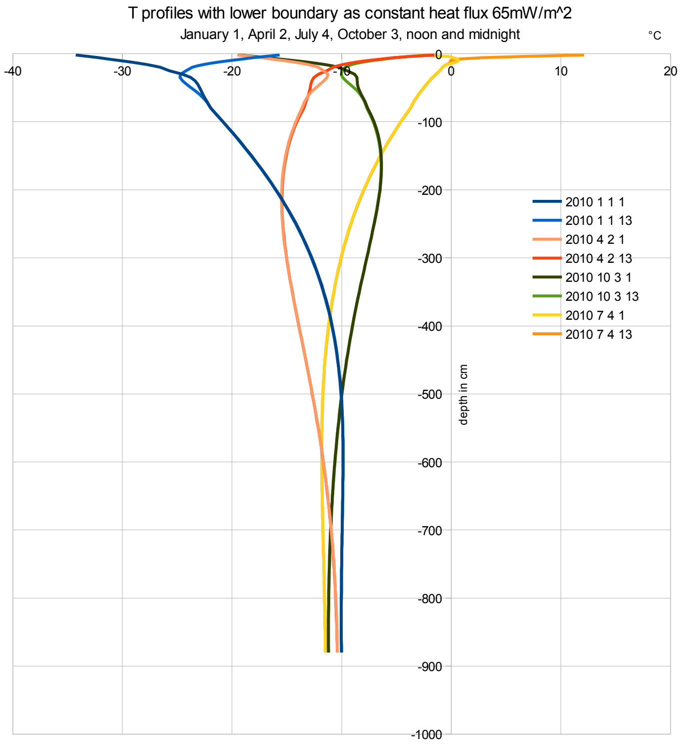

Figure 20: T-profile with initial T of -9.478°C and constant heat flux of 65mW/m^2 as lower boundary condition

Heat transfer example for unsaturated soils

If a freezing soil is not fully water saturated, the amount of energy set free by freezing the contained water is much smaller and vice versa, when thawing the soil, the required energy to thaw the soil is much smaller than for a saturated soil. This has some consequences on the duration of the freezing/ thawing process and hence on the temperatures in the upper soil layers. Since an unsaturated soil also freezes at deeper temperatures (see equation (2.24.10)) the temperature profiles show some differences compared to saturated frozen soils.

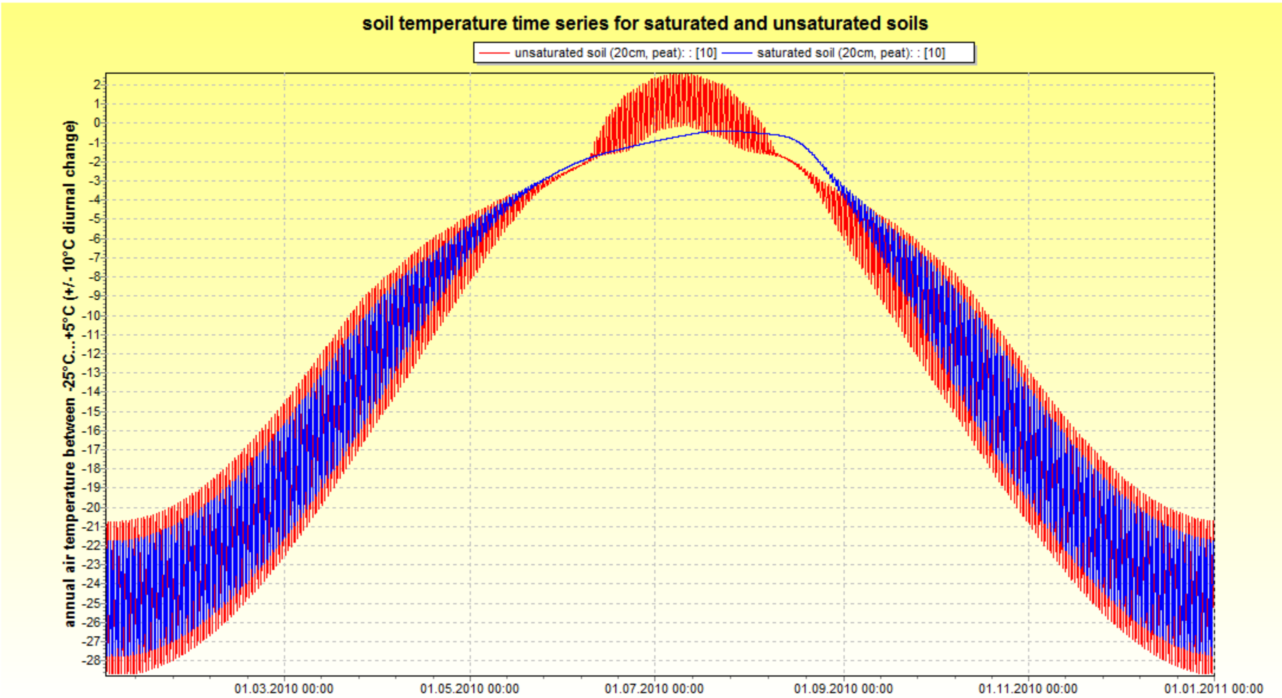

Figure 21: Comparison of soil temperatures in 20 cm depth for a saturated (blue) and unsaturated (red) peat (porosity 0.8);

Figure 21 shows a comparison between a saturated (blue) and an unsaturated (red) soil, each in 20cm depth, simulated with identical temperature input (see figure 16). The soil profile is a silty clay with a 20cm peat layer on top. Note that for unsaturated soil the melting temperature of the soil water is around -1.8°C (below and above, the large fluctuations show that there is no more ice to thaw) whereas for the saturated soil the melting temperature is sharply below 0°C (no fluctuations to bee seen because there is still ice to be molten). The generally larger diurnal fluctuations of the temperatures in the unsaturated soil are because of the lower total heat capacity (lower water content).

Figures 22 and 23 show the respective temperature curves in 45 cm and 100 cm depth. Because of the larger water content, the thermal inertia of the saturated soil is much higher – which is manifested by the lesser temperature reached in summer and the slower cool down in fall.

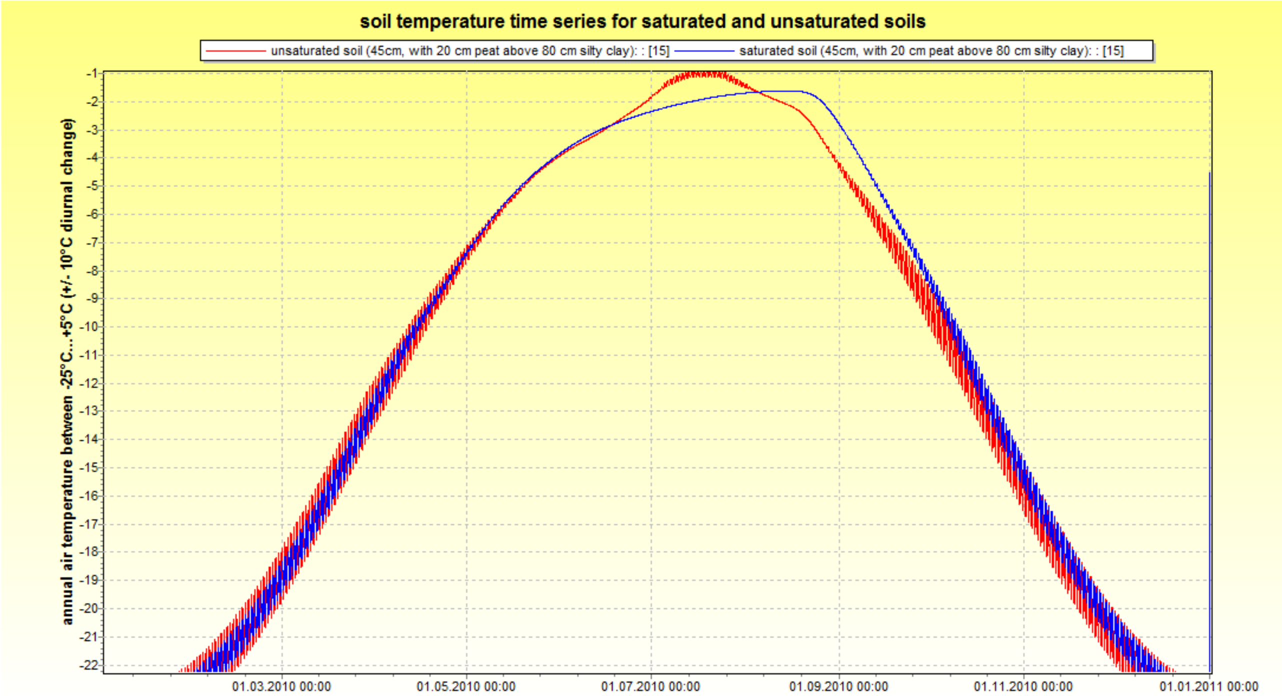

Figure 22: Comparison of soil temperatures in 45 cm depth for a saturated (blue) and unsaturated (red) soil with 20 cm peat (porosity 0.8) above 25 cm silty clay

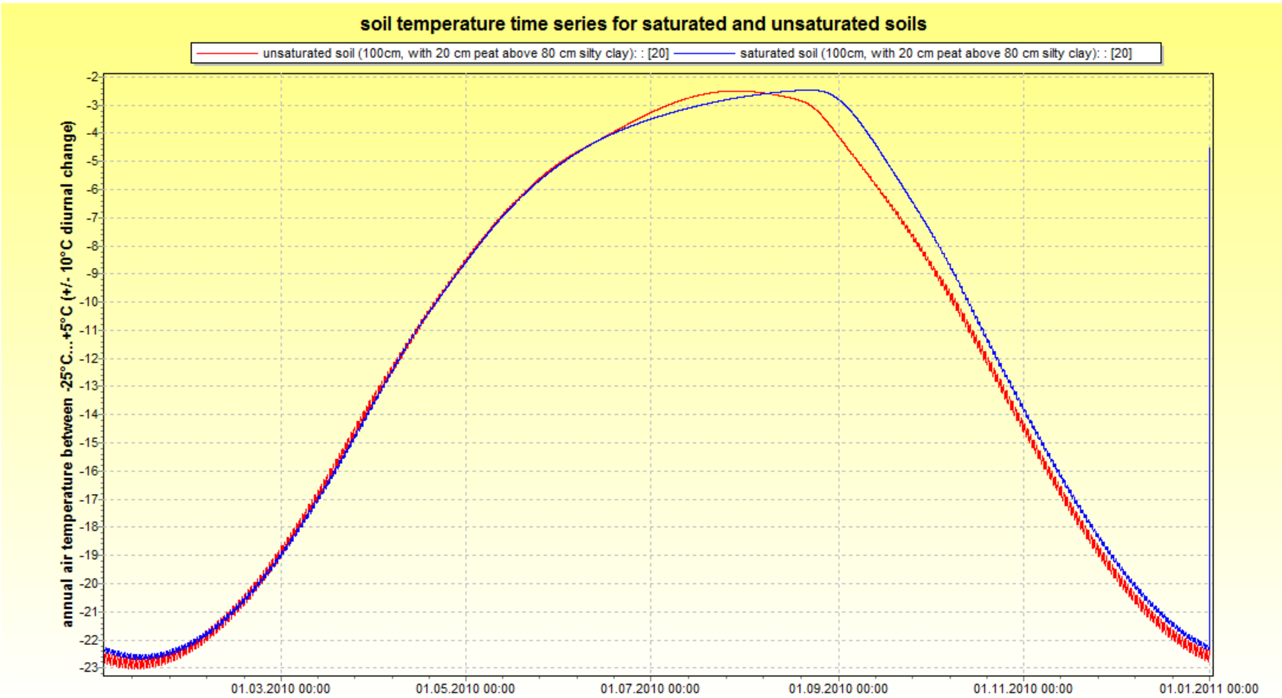

Figure 23: Comparison of soil temperatures in 100 cm depth for a saturated (blue) and unsaturated (red) soil with 20 cm peat (porosity 0.8) above 80 cm silty clay

An experiment with a very dry peat vs. a saturated peat

Finally, the temperature profiles for saturated and unsaturated soils will be compared, see figures24, 25 and 26. While figure 24compares the time series of soil temperatures in 1m depth for saturated and unsaturated conditions, figure 25 and 26 show the temperature profiles for the same two model runs (again for 4 days of the year, this time the first days of January, April, July and October). Here, the uppermost 1.0 m of the soil is a peat, either saturated (water content 0.8) or unsaturated (water content ~0.19, which is near residual water content). The temperature input is the same as used for the experiments above (see figure 16).

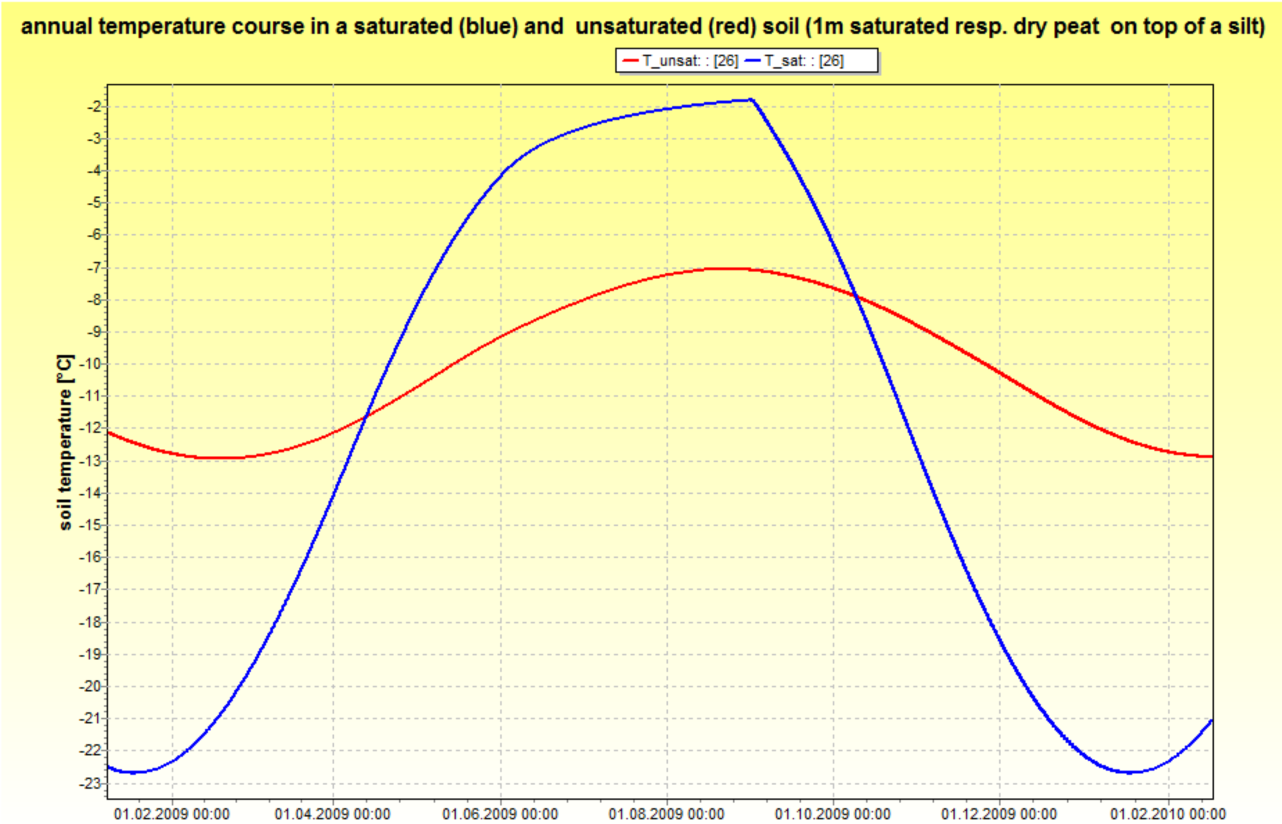

Figure 24: temperature time series in a saturated (blue) and unsaturated (red) soil in 1m depth; the soil has a 1m peat layer on a silt. For dry peat, the groundwater is at about -1.3m. No rain, no snow, no evaporation has been regarded in this experiment, only temperature as given in the examples above

It can be seen that the unsaturated soil stays much warmer in winter and cooler in summer since the dry peat is insulating the soil from the air quite efficiently. Thus, the warming from below with 130mW/m^2 shows its effect on the unsaturated soil more than on the saturated soil: since the heat loss in winter is not as high as in the saturated case, the soil is generally warmer.

Below -10m, the thermal gradient is stable (no significant annual fluctuations). This example was calculated with a constant heat flux of 130mW/m^2, which is typical for some arctic regions in Alaska (world average is around 65mW/m^2 but the range may vary considerably)

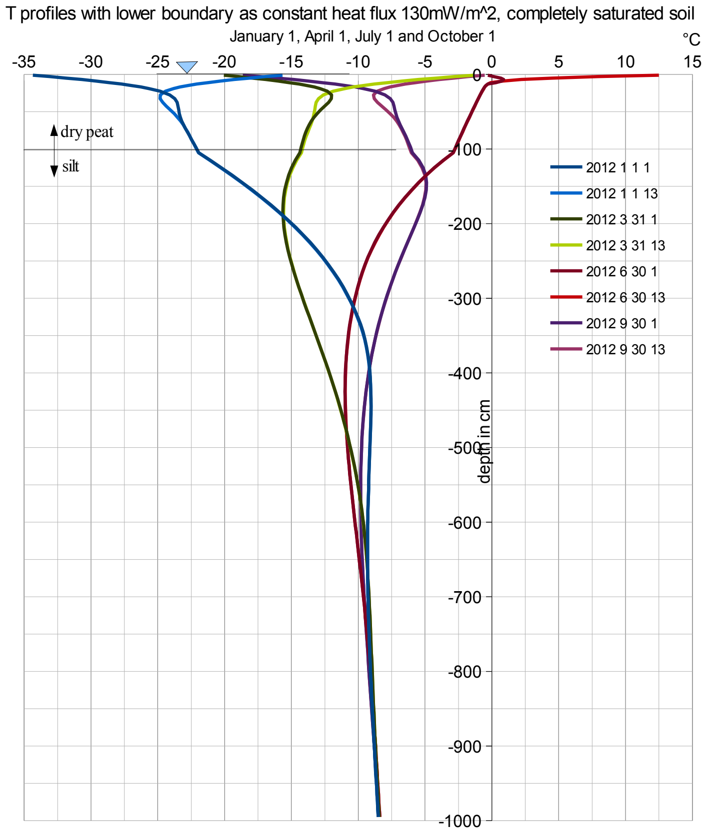

Figure 25 T-profiles for saturated soil

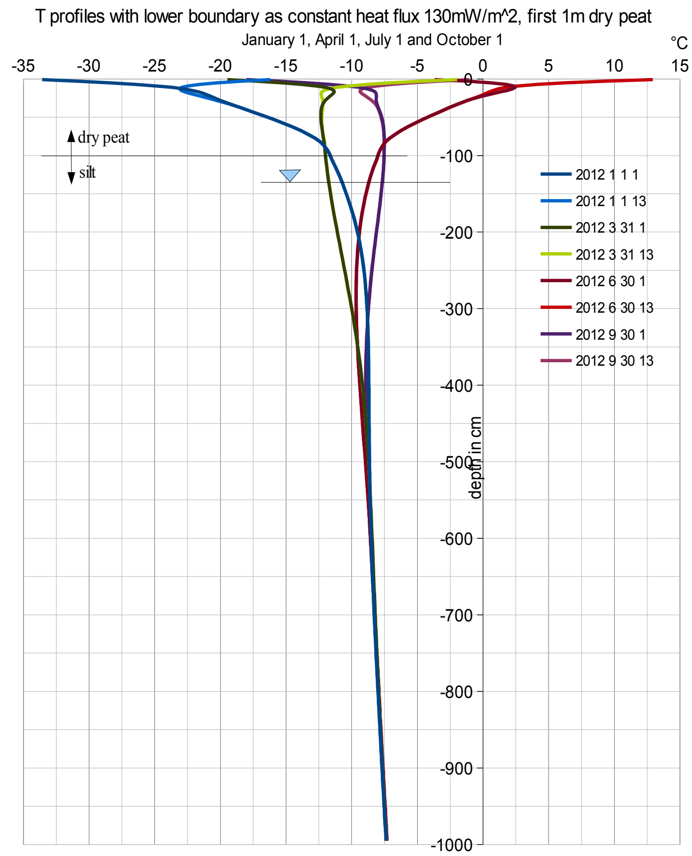

Figure 26: T-profiles for unsaturated soil

Setting up the heat transfer model in the control file

There are of course a few parameters to be defined in the control file. First of all, there is a new section called [heat_transfer]. Here, all temperature modelling related parameters must be defined. In addition, some parameters can be set in the soil table to individual values per soil, overriding the global settings in the [heat_transfer] section. The following example explains the changes in the control file in detail (rows ending with ↵ have a line break for this documentation only. In real control files, the single parameters must follow each other without empty lines):

```
# set a variable where all the other variables are set
$set $T_lower_boundary_grid =  $grid//.tlowbdry

# also, a variable may be defined for the result-stack for temperatures and another
#one for the grid with the active layer thickness (thaw depth)
$set $Temperaturestack  = tsoil//stack//.//$suffix
$set $ThawDepthGridTMod = thaw//$grid//.//$suffix

# an optional standard grid for the lower boundary condition may be defined here.
# if the boundary condition should change over time (e.g. because the soil depth is not
# deep enough to suppress intra-annual fluctuations), a series of boundary condition
# grids may be supplied, using the periodicity and persistent tags:
# periodicity = 30 D 24 persistent = 1
[standard_grids]
$inpath_grid//$T_lower_boundary_grid    T_Lower_Boundary_Condition fillcode = 1
defaultValue = -10 writecode = 8 readcode = 0 # periodicity = 30 D 24 persistent = 1


# the following section for heat transfer can be used with WaSiM version 9.0 ff
[heat_transfer]
1  # 0 = do not model heat transfer, 1 = heat transfer is modelled
11 # vertical 1D heat transfer in the unsaturated zone (0=no, 1=yes using explicit time↵
        stepping, only heat diffusion,  2 = yes, heat diffusion and convection (by ↵
        infiltrating water, not yet available)), 11 = only diffusion but using an ↵
        implicit solution scheme,12 = diffusion and convection with implicit solution ↵
        scheme (not yet implemented)
0  #  vertical heat transfer in snow cover (not yet available)
0  #  2D lateral heat transfer by advection (coupled to water transport) in ↵
        groundwater (not yet available)
# parameters
# the lower boundary condition for temperature may either be defined by a grid with ↵
the internal name _T_Lower_Boundary_Condition_ or created by using the annual ↵
temperature and the lapse rate as defined in the next two lines ↵
-10.0   # used when no grid "_T_Lower_Boundary_Condition_" was read in only: mean annual
↵ air temperature reduced to sea level to be used as lower boundary condition (e.g. 5°C)
↵ --> used for definition of the lower boundary condition at lower soil boundary, if no
↵ grid with lower boundary condition was read in
-0.007  # used when no grid "_T_Lower_Boundary_Condition_" was read in only:
temperature↵ gradient (e.g. -0.007 K/m) for defining the lower boundary condition (used
if no grid↵ with lower boundary condition was found)
# default soil "constants": can be changed in the soil table (using DryHeatCapacity,↵
DryDensity and DryThermalConduct as parameter names)
800     # default heat capacity of dry soil in J/(Kg*K), default 800 --> value may be↵
given in detail for each soil type in the soil table
1500    # default density of dry soil in Kg/m^3 , default 1500 --> value may be given
in↵ detail for each soil type in the soil table
0.58    # default thermal conductivity for dry soil in J/(m*s*K) or W/(m*K): ↵
default: 0.58 --> value may be given in detail for each soil type in the soil table
1e-11     # reduced k_sat (minimum hydraulic conductivity for fully frozen soils)
# thermodynamic constants of water and ice (not for calibration! these are constants
giving only marginal room for variations)
0.5562  # thermal conductivity of liquid water (do not change, this is a matter
constant)
2.33    # thermal conductivity of ice (0°C...-20°C) do not change either
4187    # heat capacity of water in J/(Kg*K) do not change as well
1940    # heat capacity of ice at -20°C in J/(Kg*K) should also not be changed
```

```
2090    # heat capacity of ice at 0°C in J/(Kg*K) also please do not touch the value
334000  # latent heat of freezing in J/Kg this is a constant, please do not change
1000    # density of water in Kg/m^3 rather a constant (for our reasons). Do not touch!
# other parameters (not for calibrating, but there is no clear lioterature value)
1.22    # scaling factor (solution of the clapeyron equation, literature gives values
of↵ 1.8 up to 123, bhut this may be measure dependent. Theoretical value ↵
is dH/T_m = 1.22 J/(Kg*K))
0.8     # SE value which must be underrun to evaluate the soil layer as frozen for the↵
Thawdepth-output grid and statistics
60      # minimum sub time step allowed for heat transfer model (numeric errors like↵
extreme temperature fluctuations are possible if the value is too large)
1200    # maximum sub time step allowed for heat transfer model (to avoid instabilities↵
induced by the non-linearity of the processes)
1.0     # n-factor for freezing (factor applied to the air temperature to get the↵
temperature at the soil surface as upper boundary condition when temperatures are↵
negative
1.0     # n-factor for thawing (factor applied to the air temperature to get the↵
temperature at the soil surface as upper boundary condition when temperatures are↵
positive
# output grids and statistics
$outpath//ts_loc//$grid//.//$year # results soil temperature for control point
$outpath//ts_avg//$grid//.//$year $once_per_interval # results soil temperature↵ thaw
depth or active layer thickness as average value for subbasins
$outpath//$Temperaturestack  # stack, actual soil water content for all soil levels
$Writegrid                   # Writecode for this stack
$outpath//$ThawDepthGridTMod # output grid containing the active layer thickness
$Writegrid                   # Writecode for this stack
$readgrids                             # like in all other models: 1 = read stack for
temperature,↵  0 = create new stack according to boundary conditions (linear
interpolation between↵ upper and lower boundary condition)

[soil_table]
1                   # number of following entries
7 silty_clay_(SIC) {method = MultipleHorizons;
....
 DryHeatCapacity        = 810  # dry heat capacity in J/(Kg*K)
 DryDensity             = 1450 # dry density in m^3/m^3
 DryThermalConduct      = 0.57 # dry thermal conductivity in W/(m*K) (or J/(m*s*K)
 KMinFrozenSoil = 1e-12 # minimum hydraulic conductivity in m/s when the soil is
#completely frozen (do not set to zero, since the logarithm of this value is used
#internally)
...
}

# alternatively, some parameters can be provided per horizon:
[soil_table]
1                   # number of following entries
7 silty_clay_(SIC) {method = MultipleHorizons;
....
KMinFrozenSoil  = 1e-12 # minimum hydraulic conductivity in m/s when the soil is ↵
#completely frozen (do not set to zero, since the logarithm of this value is used ↵
#internally)
horizon                 = 1     2       3    ; # ID of the horizon
Name                    = Peat  SIC10m  something ;  # short descriptions
DryHeatCapacity = 810   800     900   ; # dry heat capacity in J/(Kg*K) per horizon
DryDensity              = 450   900     1450 ; # dry density in m^3/m^3  per horizon
DryThermalConduct       = 0.3   0.5     0.57 ; # dry thermal conductivity in W/(m*K)
per  horizon
...
}

[landuse_table]
2
1  peat_landscape {method = VariableDayCount;
RootDistr         = 1.0;
TReduWet          = 1.0;
LimitReduWet      = 0.5;
HReduDry          = 3.5;
IntercepCap       = 0.3;
JulDays           = 15   46   74   105  135  166   196   227   258   288   319   349 ;
```

```
Albedo           = 0.2  0.2  0.2  0.2  0.2  0.2   0.2   0.2   0.2   0.2   0.2   0.2 ;
rsc              = 100  100  100  100  100  100   100   100   100   100   100   100 ;
rs_interception  = 100  100  100  100  100  100   100   100   100   100   100   100 ;
rs_evaporation   = 150  150  150  150  150  150   150   150   150   150   150   150 ;
LAI              = 1    1    1    1    1    1     1     1     1     1     1     1   ;
Z0               = 1    1    1    1    1    1     1     1     1     1     1     1   ;
VCF              = 0.5  0.5  0.5  0.5  0.5  0.5   0.5   0.5   0.5   0.5   0.5   0.5 ;
RootDepth        = 0.4  0.4  0.4  0.4  0.4  0.4   0.4   0.4   0.4   0.4   0.4   0.4 ;
AltDep           = 0    0    0    0    0    0     0     0     0     0     0     0   ;
n-factor            = 0.8  0.8  0.9  0.9  0.9  1.0   1.0   1.0   1.2   1.0   0.8   0.8 ;
# factor applied to the air temperatur to estimate the soil surface temperature as
# boundary condition for the soil temperature. Values are interpolated and not altitude
# corrected
}
```

Additional remarks

The hydraulic conductivity of the aquifer in the groundwater model will be adjusted for frozen layers. To do this, only the saturated soil layers are examined for their temperatures. If a layer is frozen, the transmissivity for this layer is accordingly set (hydraulic conductivity for frozen soil after equation (2.24.8c) times layer thickness). All layers' transmissivities are then integrated (transmissivities added up) over the entire saturated soil (frozen and unfrozen) and the result is divided by the total saturated (frozen and unfrozen) thickness and set as new effective hydraulic conductivity for the groundwater model.