Ch. 5: Heat Transport

Table of Contents

5 Heat Transport

5.1 Introduction

The importance of soil temperature

Soil temperature is a factor of primary importance for several processes related to transformation and transport of matter in the soil plant atmosphere system. In particular, temperature strongly influences biological processes such as root growth and microbial transformation of carbon and nitrogen in soil as well as pesticide breakdown. Thus, a soil temperature model has been developed to provide soil temperature for abiotic functions governing several biological processes described in other submodules of Daisy.

Soil temperature profile

Soil temperature varies in response to the radiant, thermal and latent energy exchange processes, which take place primarily through the soil surface. These phenomena propagate into the soil profile by a complex series of processes, the rate of which is affected by time-variable and space-variable soil properties. The pertinent soil parameters include heat capacity and thermal conductivity, both of which are strongly affected by soil texture, soil mineralogy, soil bulk density and soil water content.

Heat flow by conduction and convection

The present soil temperature model is based upon the one dimensional heat flow equation, which takes into account heat flow due to conduction and convection. Furthermore, the heat flow equation is expanded to include frost as well as thaw processes. The thermal parameters of soil are calculated on the basis of the composition of the soil and the properties of the individual constituents.

5.2 Heat flow equations[1]

The one dimensional heat flow equation

The combined one dimensional heat flow is given by:

$$q_h = -K_h \frac{\partial T}{\partial z} + c_w T q_w \qquad (5.1)$$

q_h = heat flux density [W m^{-2}]

K_h = thermal conductivity [W m^{-1} K^{-1}]

T = temperature [K]

z = depth [m]

c_w = volumetric heat capacity of water [J m^{-3} K^{-1}]

q_w = water flux density (Darcian) [m s^{-1}].

The first term of eq. (5.1) represents heat flow due to conduction and the second term due to convection.

Conservation of soil heat is described by equation (5.2):

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[1] The inclusion of freezing and thawing in these equations is rather unstable, and the default setting of the model is to not include these processes. This part of the model awaits a review. The original process descriptions are found in Hansen et al. (1990).

$$\frac{\partial H}{\partial t} = -\frac{\partial q_h}{\partial z} + S_h \tag{5.2}$$

H = heat content of soil [J m^{-2}]

t = time [s]

S_h = heat sink/source terms [J m^{-2} s^{-1}].

Assuming no latent heat due to fusion or evaporation, the change in heat content can be expressed by:

$$\frac{\partial H}{\partial t} = \frac{\partial (C_s T)}{\partial t}$$

$$= C_s \frac{\partial T}{\partial t} + \frac{\partial C_s}{\partial t} T \tag{5.3}$$

C_s = volumetric heat capacity of soil [J m^{-3} K^{-1}]

Neglecting the influence of soil air on heat capacity and no presence of ice, the change in volumetric heat capacity can be expressed as:

$$\frac{\partial C_s}{\partial t} = \rho_w c_w \frac{\partial x_w}{\partial t} = \rho_w c_w \frac{\partial \theta}{\partial t} \tag{5.4}$$

However, we know from Richards equation (eq. X.XX) that:

$$\frac{\partial \theta}{\partial t} = \frac{\partial q_w}{\partial z} - S_w \tag{5.5}$$

where S_w is the volumetric water sink [m^3 m^{-3} s^{-1}].

Combining equations (5.3), (5.4) and (5.5) results in:

$$\frac{\partial H}{\partial t} = C_s \frac{\partial T}{\partial t} - c_w \frac{\partial q_w}{\partial z} T - c_w \rho_w S_w T \tag{5.6}$$

Merging equation(5.1), (5.2) and (5.6) and assuming that $S_h = -\rho_w c_w S_w T$ we get

$$C_s \frac{\partial T}{\partial t} - c_w \frac{\partial q_w}{\partial z} T - S_h = \frac{\partial}{\partial z}\left(K_h \frac{\partial T}{\partial z}\right) - c_w \frac{\partial q_w T}{\partial z} + S_h$$

or

$$C_s \frac{\partial T}{\partial t} = K_h \frac{\partial^2 T}{\partial z^2} + \frac{\partial K_h}{\partial z} \frac{\partial T}{\partial z} - c_w q_w \frac{\partial T}{\partial z} \tag{5.7}$$

5.3 Heat capacity of soil

The volumetric heat capacity of a unit volume of soil can be estimated by addition of the heat capacity of the various constituents of the soil.

$$C_s = x_m \rho_m c_m + x_q \rho_q c_q + x_o \rho_o c_o + x_w \rho_w c_w + x_a \rho_a c_a \qquad (5.8)$$

Where

C_s = volumetric heat capacity [J m^{-3} K^{-1}] of the soil

c = specific heat capacity [J kg^{-1} K^{-1}] of each material

ρ = density [kg m^{-3}] of each material

x = fraction (for liquid water equal to volumetric water content θ)

and subscripts are

a = air

m = mineral particles, not quarts

o = organic particles

q = quarts particles

w = liquid water

$$x_m + x_q + x_o + x_w + x_a = 1 \qquad (5.9)$$

The specific heat capacity and the density of the different constituents are given in Table 5.1.

Table 5.1. Density (ρ), specific heat capacity (c), and thermal conductivity (K) of different soil constituents. Water and air at 10°C (de Vries, 1963).

Soil constituents	ρ kg m^{-3}	c J kg^{-1} K^{-1}	K W m^{-1} K^{-1}
Quarts	2660	750	8.8
Clay minerals	2650	750	2.9
Organic matter	1300	1920	0.25
Water	1000	4192	0.57
Ice	920	2050	2.2
Air	1.25	1005	0.025

Most soil minerals have about the same densities and specific heats (de Vries, 1963), therefore the different soil mineral constituents are pooled. From Table 5.1 it is evident that the contribution of air to the volumetric heat capacity of the soil can be neglected. The amount of quarts in a soil horizon can be estimated from soil texture based on Moberg et al. (1988) (for Danish soils):

$$\frac{x_q}{x_q + x_m} = clay * 0.15 + silt * 0.6 + sand * 0.7 \qquad (5.10)$$

$clay$ = fraction of mineral particles < 2µm

$silt$ = fraction of mineral particles between 2 and 63 µm

sand = fraction of mineral particles between 63 µm and 2 mm.

The rest of the mineral fraction is assumed to be clay minerals. Thus, as default, the quarts fraction is calculated based on texture and the volumetric heat capacity is then calculated based on equation (5.8) every timestep.

5.4   Thermal conductivity of soil

Table 5.1 shows the thermal conductivity of various soil constituents. Thermal conductivity of a soil depends on its composition, i.e. the fractions of its different constituents, but the dependence is a very complex one. At complete dryness, the heat mainly flows through the grains around their contact points. When the soil is wet, the heat conductivity of water is mainly responsible for heat conduction. Because of the large difference in thermal conductivity between air and water, the thermal conductivity of the soil depends heavily on the water content of the soil, especially in relative dry situations when water bridges are being formed between grains.

de Vries (1952) and de Vries (1963) developed a physically based model for calculating the thermal conductivity of a soil on basis of its constituents. The model is based on an analogy to the physical problems of expressing the electric conductivity or the dielectric constant of a granular material as a function of the volume fractions and the respective physical properties of its constituents. (Burger, 1919) solved this analogous problem mathematically.

The basic ideas of the model is outlined below. Consider a volume V consisting of a continuous medium, with the volume fraction x_0 and the thermal conductivity K_0, in which N different types of granular materials with the volume fractions x_i and the thermal conductivities K_i are dispersed. The average heat flow through the volume can be calculated from Eq.(5.11).

$$q_h = \frac{1}{V}\int q dV = \frac{1}{V}\int -KG dV \qquad (5.11)$$

Where

q_h = average heat flow vector [W m^{-2}]

q = local heat flow vector [W m^{-2}]

K = local thermal conductivity [W m^{-1} K^{-1}]

G = local thermal gradient vector [K m^{-1}]

Assuming that in the same material the same gradient exists throughout the volume, the average heat flux can be calculated from Eq.(5.12).

$$q_h = \sum_{i=0}^{N} x_i K_i G_i \qquad (5.12)$$

x_i = volume fraction of material i

K_i = thermal conductivity of material i

G_i = thermal gradient in material i

When introducing an apparent thermal conductivity, K_h, the average heat flow through the volume can be calculated from eq.(5.13).

$$q_h = -K_h \bullet G_v \tag{5.13}$$

G_v = average thermal gradient given by Eq. (5.14).

$$G_v = \frac{1}{V}\int G dV = \sum_{i=0}^{N} x_i G_i \tag{5.14}$$

Combining Eqs. (5.12), (5.13) and (5.14) results in Eq. (5.15):

$$K_h \sum_{i=0}^{N} x_i G_i = \sum_{i=0}^{N} x_i K_i G_i \tag{5.15}$$

Considering the flow in the **e** direction ($|e| = 1$), Eq. (5.16) is obtained.

$$K_h \sum_{i=0}^{N} x_i G_i \bullet e = \sum_{i=0}^{N} x_i K_i G_i \bullet e$$

Or

$$K_h = \frac{\sum_{i=0}^{N} x_i K_i G_i \bullet e}{\sum_{i=0}^{N} x_i G_i \bullet e} = \frac{x_0 K_0 + \sum_{i=0}^{N} f_i x_i K_i}{x_0 + \sum_{i=0}^{N} f_i x_i} \tag{5.16}$$

$$f_i = \frac{G_i \bullet e}{G_0 \bullet e}$$

The value of f_i depends on the ratio (K_i/K_0), on the size and shape of the granules, and on their relative positions. A mathematical expression for f_i can be found under the following restrictions:

- The granules are of ellipsoidal shape
- The granules are so far apart that they do not interact.

For a grain in form of an ellipsoid with principal axes a_1, a_2, a_3, eq. (5.17) and eq. (5.18) are derived for a temperature gradient in the direction a_j (Burger, 1919).

$$f_{ij} = \left[1 + \left(\frac{K_i}{K_0} - 1 \right) g_j \right]^{-1} \tag{5.17}$$

$$g_j = \frac{1}{2} a_1 a_2 a_3 \int_0^{\infty} \left[(a_1^2 + u)(a_2^2 + u)(a_3^2 + u) \right]^{-\frac{1}{2}} (a_j^2 + u)^{-1} du \tag{5.18}$$

In the theory of the dielectric constant, the quantity g_j is called the depolarization factor of the ellipsoid in the direction of the a_j-axis. In the theory of the thermal heat conduction, g_j is often called the shape factor (de Vries, 1952; de Vries, 1963). The value of g_j depends on the ratios of the principal axis (a_j), but not on their absolute value.

$$g_1 + g_2 + g_3 = 1 \qquad (5.19)$$

If the ellipsoidal granulas are randomly orientated, then f_i is given by eq.(5.20).

$$f_j = \sum_{j=1}^{3} f_{ij} \qquad (5.20)$$

For a spheroid with the axis $a_1 = a_2 = \alpha a_3$, g_1 can be written as eq.(5.21):

$$g_1 = \tfrac{1}{2}\alpha^2 a_3^3 \int_0^\infty \left((\alpha a_3)^2 + u\right)^{-2} \left(a_3^2 + u\right)^{-\frac{1}{2}} du$$

$$= \tfrac{1}{2}\alpha^2 \int_0^\infty \frac{dV}{\left(\alpha^2 + V\right)^2 \left(1+V\right)^{\frac{1}{2}}} \qquad (5.21)$$

For $\alpha < 1$ (oblate spheroid):

$$g_i = \tfrac{1}{2}\frac{\alpha^2}{\left(1-\alpha^2\right)}\left[\frac{1}{\alpha^2} + \frac{1}{2\left(1-\alpha^2\right)^{\frac{1}{2}}}\ln\left(\frac{1-\left(1-\alpha^2\right)^{\frac{1}{2}}}{1+\left(1+\alpha^2\right)^{\frac{1}{2}}}\right)\right] \qquad (5.22)\ (a)$$

For $\alpha = 1$ (spherical granulas)

$$g_1 = \tfrac{1}{3} \qquad (5.22)\ (b)$$

For $\alpha > 1$ (prolate spheroid)

$$g_1 = \tfrac{1}{2}\frac{\alpha^2}{\left(\alpha^2 - 1\right)}\left[\frac{\pi}{2\left(\alpha^2 - 1\right)^{\frac{1}{2}}} - \frac{1}{\alpha^2} - \frac{1}{\left(\alpha^2 - 1\right)}arctg\left(\left(\alpha^2 - 1\right)^{-\frac{1}{2}}\right)\right] \qquad (5.22)\ (c)$$

For all three cases:

$$g_2 = g_1 \qquad (5.23)$$

$$g_3 = 1 - 2g_1$$

$$\qquad (5.24)$$

For elongated cylinders with elliptical cross section:

$$a_1 = ma_2$$

$$(5.25)\ (a)$$

$$a_3 = \infty$$

$$(5.25)\ (b)$$

$$g_1 = \frac{1}{m+1}$$

$$(5.25)\ (c)$$

$$g_2 = \frac{m}{m+1}$$

$$(5.25)\ (d)$$

$$g_3 = 0$$

$$(5.25)\ (e)$$

For flat particles with small thickness, lamellae:

$$a_2 = a_3 = \infty$$

$$(5.26)\ (a)$$

$$g_1 = 1$$

$$(5.26)\ (b)$$

$$g_2 = g_3 = 0$$

$$(5.26)\ (c)$$

Use of the model

For solid soil particles, the spheroid model with an α-value around 4 can often be used (de Vries, 1963). In moist soils, water can be considered a continuous medium in which soil particles and air voids are dispersed. We use water as the continuous medium down to the soil water content corresponding to half way between field capacity (pF = 2.0) and wilting point (pF = 4.2). de Vries (1963) states "In moist soils water can be considered as a continuous medium, in which soil particles and air voids are dispersed, for moisture contents ranging from saturation to well below field capacity". In dry soils, air can be considered the continuous medium. We use air as the continuous medium up to the soil water content at pF 4.2. In the region between soil water content half way between field capacity and the wilting point, the thermal conductivity is found by interpolation.

In most soils, heat transfer in the air filled pore space does not only take place as thermal conduction, but also as latent heat, i.e. transfer of heat by diffusion of water vapour in the soil air. The transfer of energy as latent heat is highly dependent on the soil temperature. At 0°C, the transfer of heat by conduction and by vapour diffusion is of the same order of magnitude. The influence on the transfer of heat as latent heat is taken into account by substituting the thermal conductivity of the air by an apparent conductivity, eq. (5.27):

$$K_a^{'} = K_a + K_v \tag{5.27}$$

$K_a^{'}$ = apparent thermal conductivity of soil air [W m^{-1} K^{-1}]

K_a = thermal conductivity of soil air [W m^{-1} K^{-1}]

K_v = thermal conductivity due to vapour transfer [W m^{-1} K^{-1}]

At moisture contents below the wilting point, the liquid is held by adsorption forces and the relative humidity becomes considerably less than 1. Then the transfer of heat by water vapour is restricted. We assume that the thermal conductivity due to vapour diffusion can be estimated from eq. (5.28):

$$K_v = \begin{cases} K_v^s \dfrac{\theta}{\theta_{wp}} & \text{for } \theta < \theta_{wp} \\ K_v^s & \text{for } \theta \geq \theta_{wp} \end{cases} \tag{5.28}$$

K_v^s = thermal conductivity due to vapour diffusion under saturated conditions [W m^{-1} K]

θ = volumetric soil water content [m^3 m^{-3}]

θ_{wp} = volumetric soil water content at pF = 4.2 [m^3 m^{-3}]

We have used the value 0.04 W m^{-1} K for K_v^s, which is a reasonable value at a temperature around 10°C (de Vries, 1963).

Calculations with water as continuous medium

When the soil is near water saturation, soil air forms spherical voids. Figure 5.1 illustrates the influence of the shape factor (g) on the parameter (f). The minimum influence occurs when $g_1 = g_2 = g_3$ = 1/3. As the water content of the soil decrease, air replaces water and subsequently, the f-values increase. As it may be seen from Figure 5.1, this occurs at decreasing values of g_1. It is assumed that the g-values assume values which correspond to an oblate spheroid with an α-value of the order of 10 (g_1 = 0.07) at a soil water content corresponding to pF = 4.2. By assuming a linear relation between g_1 and x_a in the region of water content between the saturated condition and pF 4.2, eq. (5.29) is obtained.

$$g_1 = 0.333 - (0.333 - 0.070) \frac{x_a}{\theta_s - \theta_{wp}} \tag{5.29}$$

θ_s = saturation water content

Furthermore, it is assumed that $g_2 = g_1$ and subsequently that $g_3 = 1 - 2g_1$. It is noted that the relations only is used down to a water content corresponding to half way between field capacity (pF = 2) and wilting point (pF = 4.2).

Calculation with air as continuous medium

In the dry situation when air can be considered as the continuous medium, the water, which is present, forms a thin film covering the soil particles and small water rings around the contact points of the particles. These water rings act as bridges for the heat flow. It is assumed that water has a maximum contribution to

the heat transfer. This is obtained by setting $g_1=1$ and $g_2 =g_3 = 0$, which corresponds to flat particles with small thickness.
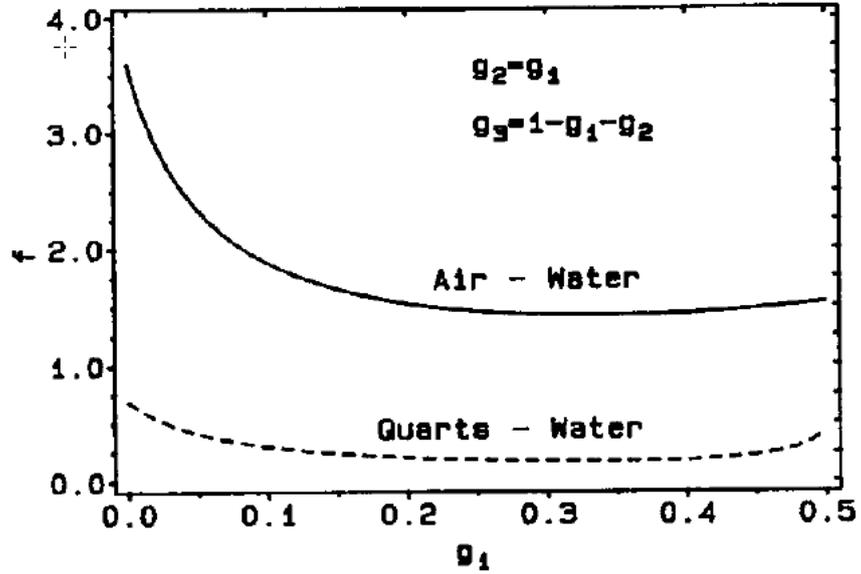

Figure 5.1. Relationships between the parameter f and the shape factor g1 for systems with water as the continuous medium and with air and granular of quarts, respectively, as dispersed material.
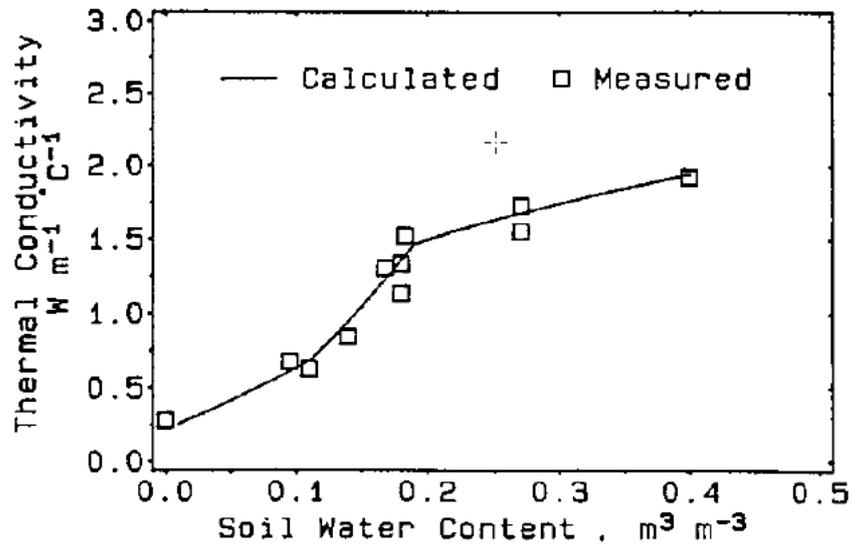

Figure 5.2- Measured and calculated thermal conductivity of soil related to soil water content. The experimental data stem from (Mogensen, 1969) and calculations were carried out with de Vries' model assuming a porosity of 40 %, a quarts fraction of 30 %, a fraction of other minerals of 27 % and an organic fraction of 3 %. The form factor of solid particles (quarts and other minerals) corresponded to spheriodes with an α-value equal to 3.5 (eq. (5.22)(c)), and that the form factor of the organic material corresponded to elongated cylinders with elliptical cross section (m=3 in eq. (5.24)). The field capacity is 0.27 and the wilting point is 0.11.

5.5   Boundary conditions [coordinate with Ch.2]

Soil surface temperature is assumed to constitute the upper boundary condition of the default SVAT model (see the SSOC-model for another approach). The soil surface temperature is approximated by the air temperature except when snow is covering the soil surface. If infiltration is due to irrigation, it is assumed that the infiltrating water assumes the temperature of the irrigation water.

If hourly air temperature values are available, these are used directly. To include a diurnal variation in the air temperature when daily min-max temperature values are available, it is assumed that the minimum temperature occurs just before sunrise and maximum temperature occurs at 15.00 hours, if the average daily temperature is higher than the temperature of the previous night. If the average daily temperature is lower than the temperature of the previous night, it is assumed that the minimum temperature of the day occurs at 9 a.m.

If snow is present and the snow contains liquid water, it is assumed that the surface temperature is 0°C. If snow is present ant the snow does not contain any liquid water, the surface temperature (the temperature at the bottom of the snow) is calculated by assuming steady state heat flow through the snow cover and through the upper soil, that is:

$$-K_s \frac{T_{sf} - T_a}{\Delta z_s} = -K_{h1} \frac{T_1 - T_{sf}}{z_1}$$

Or

$$T_{sf} = \frac{(K_{h1}/z_1)T_1 + (K_s/\Delta z_s)T_a}{(K_{h1}/z_1) + (K_s/\Delta z_s)} \quad (5.30)$$

T_{sf} = surface temperature [K]

T_a = air temperature [K]

T_1 = soil temperature at z_1 [K]

z_1 = soil depth [m]

Δz_s = depth of snow cover [m]

K_{h1} = thermal conductivity of soil [W m^{-1} K^{-1}]

K_s = thermal conductivity of snow [W m^{-1} K^{-1}].

The thermal conductivity of snow is estimated according to (Corps of Engineers, 1956):

$$K_s = S\rho_s^2 \quad\quad (5.31)$$

S = empirical parameter [2.86 · 10^{-6} W m^4 kg^{-2}]

ρ_s = density of snowpack [kg m^{-3}].

Subsoil irrigation water   Subsoil irrigation water is assumed to have soil temperature when entering the soil.

Lower boundary   Neglecting frost, thaw and transfer of heat by convection and assuming constant C_s and K_h, eq. (5.7) is reduced to:

$$C_s \frac{\partial T}{\partial t} = K_h \frac{\partial^2 T}{\partial z^2} \tag{5.32}$$

This equation can be solved analytically with the boundary conditions given below:

$$T(t,0) = T_{av} + A_t \cos\left(\omega(t - t_0)\right) \tag{5.33}$$

$$T(t,\infty) = T_{av}$$

The solution is eq.

$$T(t,z) = T_{av} + A_t e^{-z/d} \cos\left(\omega(t - t_0) - z/d\right) \tag{5.34}$$

$$d = \left[\frac{2K_h}{C_s \omega}\right]^{1/2}$$

d is the damping depth [m]

Eq. (5.34) is used as lower boundary condition with

T_{av} = annual average of air temperature [°C]

A_t = amplitude of the annual variation in air temperature [°C]

ω = $2\pi/365$ [day^{-1}]

t = day in the year [day]

t_0 = day number when $T(t,0) = T_{av} + A_t$ [day]

K_h = average thermal conductivity of the soil profile [W m^{-1} K^{-1}]

C_s = average volumetric heat capacity of the soil profile [J m^{-3}]

z is chosen as the deepest computational point.

5.6   Parameter overview

Table 5.2. Related Parameter names in Daisy.

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default value	Default unit
α	For quarts (oblate spheroid)	HorHeat	*quarts_form_factor*	2	[]
	For minerals (oblate spheroid)	HorHeat	*mineral_form_factor*	4	[]
x_q	Fraction of quarts in soil minerals. By default, calculated from soil constituents:	Horizon	*quarts*	By default, calculated from soil constituents, eq. **Error! Reference source not found.**	[]
x_m	Fraction of minerals in soil minerals			Total mineral fraction minus quarts	[]
x_o	Fraction of organic matter	Horizon	*humus*	none	[]
	Volumetric heat capacity of dry soil (mineral, organic matter and air fractions)	HorHeat	*C_soil*	By default calculated from soil constituents, but can be specified	$[\text{erg/cm}^3/\text{dg C}]= 10^{-1}*\text{J m}^{-3}\text{ K}^{-1}$ $1 \text{ erg} = 10^{-7}\text{ J}$
	Heat conductivity table for water contents above wilting point (See Figure 5.2)	HorHeat	*K_water*	By default calculated from soil constituents, but can be specified	$[\text{erg/s/cm/dg C}]$ $10^{-5}\text{ J s}^{-1}\text{ cm}^{-1}\text{ K}^{-1}$
	Number of numeric intervals to use in the heat conductivity table	HorHeat	*intervals*	100	
	Density, specific heat capacity and thermal			Values in Table 5.1 are hard-coded.	

Name and explanation		Model (in Daisy)	Parameter name (Daisy reference manual)	Default value	Default unit
	conductivity of single soil constituents.				
Lower boundary condition					
T_{av}	Annual average of air temperature	Daisy weather file	*TAverage*	none	[°C]
A_t	amplitude of the annual variation in air temperature	Daisy weather file	*TAmplitude*	none	[°C]
t_0	day number when $T(t,0) = T_{av} + A_t$	Daisy weather file	*MaxTDay*	none	[day]
	The three parameters may be calculated by a weather program available with the model, based on a Fourier transformation analysis of the temperature data, see Appendix 5.1.				

Original text from	A10	
Updated by	date	For Daisy version
Styczen, M	2020 11 12	5.93

5.7　References

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