

# Ch. 3: Surface phenomena

## Table of Contents

|       |   |    |
|-------|---|----|
| 3     | Atmospheric environment and surface phenomena ..... | 2  |
| 3.1   | Introduction.....                                   | 2  |
| 3.2   | Modelling (free) water above ground .....           | 3  |
| 3.2.1 | Model for snow accumulation and melting .....       | 4  |
| 3.2.2 | Canopy interception model.....                      | 8  |
| 3.2.3 | Litter layer .....                                  | 10 |
| 3.2.4 | Ponding and runoff.....                             | 12 |
| 3.3   | Soil evaporation and Transpiration .....            | 14 |
| 3.3.1 | SVAT-models.....                                    | 14 |
| 3.3.2 | The uncoupled approach.....                         | 15 |
| 3.4   | Heat transport in above-ground compartments.....    | 17 |
| 3.4.1 | Concepts .....                                      | 17 |
| 3.4.2 | Calculations .....                                  | 17 |
| 3.5   | Solute transport in above-ground compartments ..... | 19 |
| 3.5.1 | An overview .....                                   | 19 |
| 3.5.2 | Definition of a chemical.....                       | 21 |
| 3.5.3 | Input of chemicals above the soil surface .....     | 21 |
| 3.5.4 | Solutes in snow.....                                | 22 |
| 3.5.5 | Solute on canopy .....                              | 23 |
| 3.5.6 | Solute in litter .....                              | 24 |
| 3.5.7 | Solute on the surface.....                          | 25 |
| 3.6   | Parameter overview .....                            | 26 |
| 3.7   | Appendices .....                                    | 31 |
| 3.8   | References.....                                     | 31 |

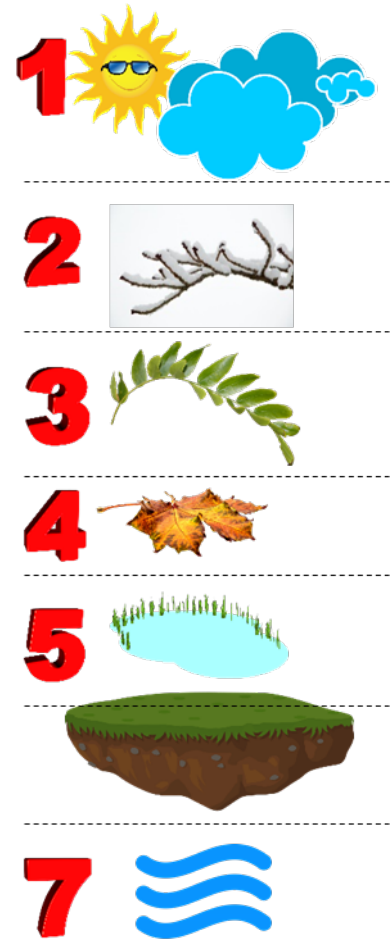
### 3 Atmospheric environment and surface phenomena

#### 3.1 Introduction

As described in Chapter 1, the Daisy model consist of several strictly ordered **compartments**, from top to bottom:

1. The atmosphere, or weather layer, described in Chapter 2.
2. The snow pack.
3. The canopy.
4. The litter layer.
5. The surface, including ponded water.
6. The soil, described in chapters 4-9.
7. The lower boundary, such as groundwater or aquifer, described together with the soil in chapter 4-9.

This chapter deals with the flow of water, heat, and solutes between the top 6 compartments, from atmosphere (1) to soil (5), as well as the internal structure of compartment 2-5, e.g., snowpack, canopy, litter, and ponding. Furthermore, the distribution of short-wave radiation within the canopy layer is described in section 10.5.



Water movement above ground is described in Section 3.2. There are three sources of liquid water: rain, management operations, and melting snow. **Liquid water** above ground only moves in one direction, downwards, between the above ground compartments. Only the optional mulch model (appendix 3.1) allows capillary rise. The snowpack, canopy, and litter compartments each have a dynamic capacity, based on the amount of snow, leaves, or crop residuals in the system. Once the capacity is reached, excess water spills off to the next layer. The canopy and litter layers also have dynamic coverage (over time), allowing water to bypass the layers entirely. From the surface layer, water may run off, evaporate, or infiltrate into the soil as part of the upper boundary for soil water flow (Chapter 4).

The **water temperature** (Section 3.4) in the snowpack, canopy, litter, and pond, are just simple mixes of the temperature of the water sources. Rain is assumed to be at air temperature, melting snow is assumed to be at 0 °C, and irrigation water temperature is by default air temperature, but can be specified by the user. The water in each of the four compartments will not be cooled down or warmed up by air or radiation.

**Above ground chemicals** (Section 3.5) follows water downward, with some important caveats: 1) chemicals may sorb to the canopy or litter layer, and 2) chemicals in ponded water may sorb to or desorb from the topsoil and 3) chemicals can be released from topsoil with soil colloids. Chemicals can be added in dissolved form with water or in dry form. Chemicals may enter the system as deposition from the atmosphere, by management operations, from the canopy (e.g., plant toxins) or by generation due to decomposition in the litter or soil.

Finally, liquid water may **evaporate** from the snowpack, canopy, litter, or pond, and it may evaporate from the soil through the surface or transpire from the root zone through the stomata openings in the canopy. The evapotranspiration is calculated in two phases, first a potential evapotranspiration is calculated ( $E_p$ ) based on weather data (directly or through calculation of reference evapotranspiration ( $E_r$ ) and field conditions, see Chapter 2), then an actual evapotranspiration ( $E_a$ ) is calculated based (mostly) on available water, see Section 3.3.

The calculation of actual evaporation starts from the uppermost compartment present (snow, canopy, litter, ponded water), and then from the layers below for as long as the potential evaporation is not yet fulfilled. So, rain evaporates first (never hitting the ground), then liquid water in snow, before free water on the canopy etc. Like for downward flow of liquid water, the (incomplete) coverage of the canopy layer and below that, the litter layer, allow some of the evaporation potential to bypass each of these layers. This is described in detail in section 3.2 and 3.3.

Once all liquid water is evaporated from compartments above the soil, water may be taken from the soil as transpiration and evaporation from the soil, depending on the hydraulic properties and state of the topsoil layer. These processes are described in section 3.3, Chapter 4 and Chapter 10.

If a compartment is unable to fulfil the potential evaporation, some or all of the remaining potential may be transferred to another layer (for details see Section 3.2 and 3.3). For the atmosphere and snowpack, all the unfulfilled potential is transferred to the layer below. For the litter layer, a user specified fraction, by default 0 %, of the potential is transferred to the surface layer, in the litter covered area. For transpiration from the canopy a user specified fraction, by default 60 %, of the potential is transferred to the soil layer. Any remaining evaporation potential that cannot be fulfilled is lost, meaning actual evapotranspiration will be less than the potential evapotranspiration.

### 3.2 Modelling (free) water above ground

The surface model is shown in Figure 3.1 (identical to Figure 1.2). Each of the compartments (snowpack, interception by canopy, interception by litter and ponding on the surface) will be treated separately below. If it is snowing or a

snowpack is present, then the snowpack model is activated. If this is not the case, water will hit the canopy directly (if a canopy is present) and the interception model will be activated. Percolation out of the snowpack may be intercepted by a canopy and/or a litter layer, if present, before reaching the ground with or without standing water (ponding). Canopy throughfall, (water not hitting the canopy area), is also routed to the litter layer, if present, and then to the soil surface (again with or without ponding).

As mentioned above, it is a basic assumption that free water above ground, i.e., water stored in snowpack, or intercepted or ponded water, is evaporated before soil evaporation or transpiration takes place. Another basic assumption is that the combined evapotranspiration cannot exceed the potential evapotranspiration. As default, the reference evaporation for dry conditions,  $E_r$  (calculated as described in Chapter 2) is used for free water surfaces as well as for soil evaporation/transpiration. Only if the method used for calculation of  $E_r$  allow specification of the condition 'use\_wet true' or if one of the non-standard PM – model (for measurements carried out in the field) are applied, will the  $E_r$  for wet conditions be used as boundary condition for the wet surfaces. Particularly for daily values of precipitation, wet conditions tend to overestimate evaporation.

In the following description,  $S$  is used as notation for water storage in a compartment, while  $J$  is used for water fluxes between compartments.

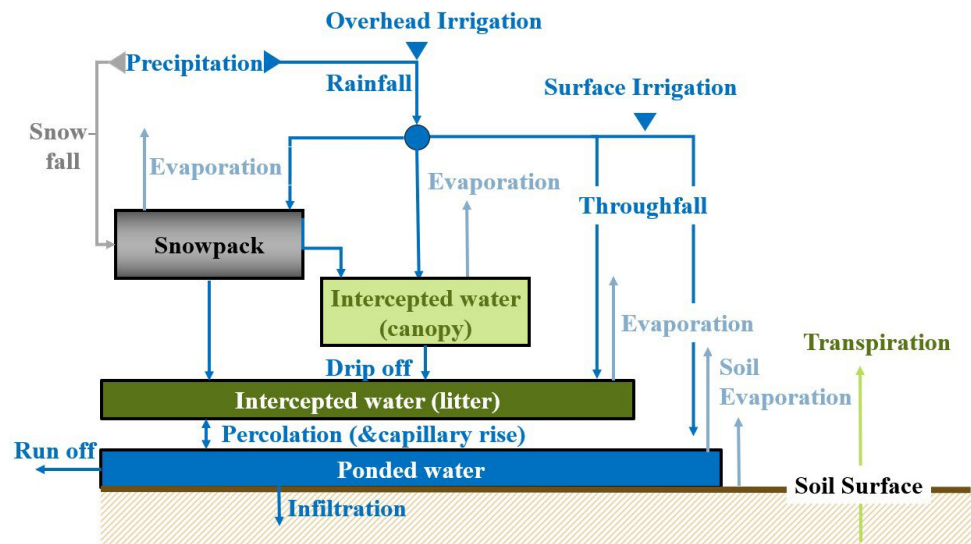


Figure 3.1. Schematic view of the water-related surface processes in Daisy (Modified from Hansen et al. (2012a))

### 3.2.1 Model for snow accumulation and melting

The model for snow accumulation is adopted from Jansson and Halldin (1980) with the modification that if ponded water occur together with a snowpack, it is considered as water in the snowpack. The basic equations in the model express the conservation of mass, e.g. of snow and water in the snow storage,  $S_{s,s}$  [mm] (Eq. 3.1) and of water in the snow storage,  $S_{w,s}$  [mm] (Eq. 3.2):

$$\frac{dS_{s,S}}{dt} = P_s + P_r + Irr^{OH} - E_s - J_{w,S} + \frac{dS_{w,Pond}}{dt} \quad (3.1)$$

$$\frac{dS_{w,S}}{dt} = P_r + M + Irr^{OH} - E_s^w - J_{w,S} + \frac{dS_{w,Pond}}{dt} \quad (3.2)$$

where

$S_{s,S}$  = snow and water in the snow storage expressed in equivalent water [mm],

$S_{w,S}$  = water in the snow storage [mm],

$S_{w,Pond}$  = surface ponding [mm], described in section 3.2.4.

$P_s$  = precipitation as snow [ $\text{mm h}^{-1}$ ],

$P_r$  = precipitation as rain [ $\text{mm h}^{-1}$ ],

$E_s$  = evaporation plus sublimation from total snow storage [ $\text{mm h}^{-1}$ ]

$E_s^w$  = evaporation from liquid water in snow storage [ $\text{mm h}^{-1}$ ],

$J_{w,S}$  = percolation from snow storage [ $\text{mm h}^{-1}$ ]

$M$  = snow melting [ $\text{mm h}^{-1}$ ], where a negative value indicates freezing.

$Irr^{OH}$  = Overhead irrigation [ $\text{mm h}^{-1}$ ]

$\Delta t$  = timestep [h]

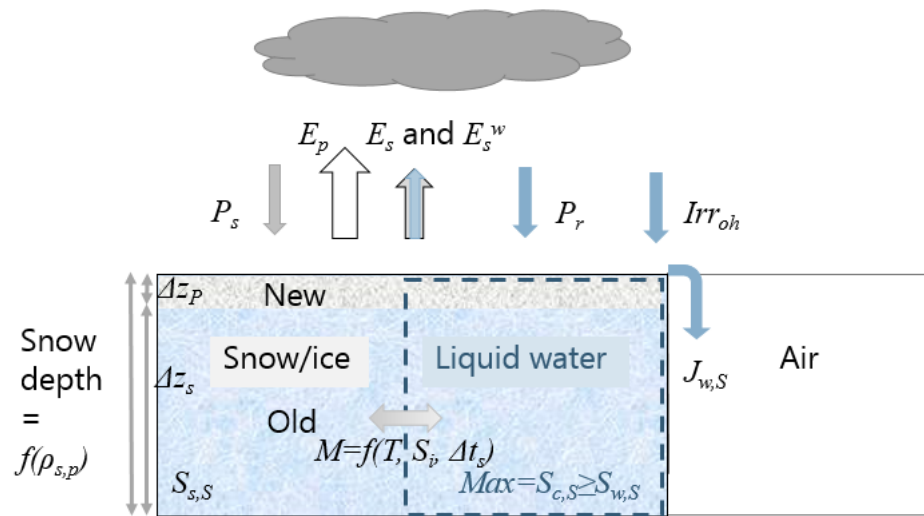


Figure 3.2. The major components of the mass balance for the snow compartment. Abbreviations as for eq. 2.1 and 2.2. Note, that  $S_{s,S}$  include both snow and liquid water while  $S_{w,S}$  contains liquid water only.  $E_s^w$  is evaporation from the liquid water fraction while  $E_s$  is the sum of evaporation and sublimation from the total snow/water storage.

## Evaporation and Sublimation

The evaporation plus sublimation from the snow storage (eq. (3.3)) and the evaporation from the liquid water in the snow storage (eq. (3.4)) are estimated as follows:

$$E_s = \begin{cases} E_p & E_s \leq P + S_{w,S}^t / \Delta t \\ P + S_{w,S}^t / \Delta t & E_s > P + S_{w,S}^t / \Delta t \end{cases} \quad (3.3)$$

$$E_s^w = \begin{cases} E_s & E_s \leq P_r + M + S_{s,S}^t / \Delta t \\ P_r + M + S_{s,S}^t / \Delta t & E_s > P_r + M + S_{s,S}^t / \Delta t \end{cases} \quad (3.4)$$

where

$E_p$  = potential evapotranspiration [mm h<sup>-1</sup>], calculated as normal reference evapotranspiration (wet or dry). The model does not consider a different albedo or height of snow.

$P$  =  $P_r + P_s$  [mm h<sup>-1</sup>].

Snow melt

The potential snow melting is assumed to be determined by the properties of the snow, the air temperature, the global radiation, and the soil heat flux at the soil surface:

$$M^* = (m_t T_a + m_r S_i + q_h / L_m) f \quad (3.5)$$

where

$M^*$  = potential snow melting [mm h<sup>-1</sup>],

$T_a$  = air temperature [°C]

$S_i$  = global radiation [J m<sup>-2</sup> h<sup>-1</sup>],

$q_h$  = soil heat flux at the surface [J h<sup>-1</sup> m<sup>-2</sup>], here always set to 0.

$L_m$  = melting heat, [J kg<sup>-1</sup>]

$m_t$  = heat sum coefficient [kg m<sup>-2</sup> °C<sup>-1</sup>·h<sup>-1</sup>], given by Eq. 3.6.

$m_r$  = global radiation coefficient [kg J<sup>-1</sup>], given by Eq. 3.9.

$f$  = constant (1 mm (H<sub>2</sub>O)/(kg (H<sub>2</sub>O) m<sup>-2</sup>)<sup>-1</sup>)

The heat sum coefficient is different for melting and freezing. Melting will affect the whole snowpack whereas re-freezing will only affect a limited surface layer. Refreezing efficiency is, therefore, inversely proportional to snow depth. The heat sum coefficient  $m_t$  is expressed by:

$$m_t = \begin{cases} m_t^* & T_a \geq 0 \\ m_t^* \cdot \text{Min} \left\{ 1; \left( (\Delta z_s + \Delta z_p) m_f \right)^{-1} \right\} & T_a < 0 \end{cases} \quad (3.6)$$

where

$m_t^*$  = constant (default value  $m_t^* = 2.0$  kg m<sup>-2</sup> day<sup>-1</sup> °C<sup>-1</sup>,

$m_f$  = constant (default  $m_f = 10$  m<sup>-1</sup>)

$\Delta z_s$  = depth of the old snowpack [m], and

$\Delta z_p$  = depth of the precipitation fallen the present day [m].

$$\Delta z_P = \frac{P \cdot \Delta t}{f \cdot \rho_P} \quad (3.7)$$

where

$\Delta t$  = time step = 1 h

$\rho_P$  = density of the newly fallen precipitation (snow-rain mixture), calculated as a weighted average of the density of water ( $\rho_w = 1000 \text{ kg m}^{-3}$ ) and powder snow ( $\rho_s = 100 \text{ kg m}^{-3}$ ):

$$\rho_P = \rho_w + (\rho_s + \rho_w) \frac{P_s}{P} \quad (3.8)$$

Albedo drops markedly with age of the snow surface, so radiation absorption increases with age. This is the reason for making  $m_r$  depending on age of the surface snow,  $\Delta t_s$ , (days since last snow fall). The influence of global radiation on snow melting and freezing in terms of the parameter  $m_r$  is expressed as:

$$m_r = m_r^* \left( 1 + m_1 \left( 1 - \exp(-m_2 \Delta t_s) \right) \right) \quad (3.9)$$

where  $m_r^*$ ,  $m_1$  and  $m_2$  are constants (default values:  $m_r^* = 1.5 \cdot 10^{-7} \text{ kg J}^{-1}$ ,  $m_1 = 2.0$  [-] and  $m_2 = 0.1 \text{ days}^{-1}$ ). To eliminate the influence of mixed precipitation and minor showers, snowfall in this context, is counted only for snowfall larger than a minimum value ( $P_{sa} = 5 \text{ mm snow per day}$ ), and a relative content of snow in the precipitation larger than 0.9 [ $f_{sa}$ ].

The actual snow melting and freezing is then estimated as:

$$M = \begin{cases} M_1 & M^* < M_1 \\ M^* & M_1 \leq M^* \leq M_2 \\ M_2 & M_2 < M^* \end{cases} \quad (3.10)$$

$$M_1 = -\left( S_{s,S}^t / \Delta t + P_r \right)$$

$$M_2 = \left( \left( S_{s,S}^t - S_{w,S}^t \right) / \Delta t + P_s \right)$$

Storage capacity for water in snow

The snow storage is assumed to possess a certain capacity for retention of liquid water which is expressed by:

$$S_{c,S} = f_c \left( S_{s,S}^t \right) \quad (3.11)$$

where

$S_{c,S}$  = storage capacity of snow storage for retention of liquid water [mm], and

$f_c$  = the capacity coefficient of snow storage for retention of liquid water, default 0.07 [-].

Percolation of water from the snow storage

The percolation of water out of the snow storage is estimated as:

$$J_{w,S} = \text{Max} \left\{ 0; S_{w,S}^t + (P_r - E_s + M + Irr^{OH}) \Delta t - S_{c,S} \right\} / \Delta t \quad (3.12)$$

The new snowpack and the new water content in the snowpack is then updated at the end of the time step according to eq. (3.1) and eq. (3.2).

Finally, the density of the snowpack is estimated. Taking compaction of the snow into consideration, a new estimate for the density of the snowpack is calculated:

$$\rho_{s,p}^{t+\Delta t} = \text{Max} \left\{ \rho_{s,p}^t; \rho_s + \rho_1 \frac{S_{w,S}^{t+\Delta t}}{S_{c,S}} + \rho_2 S_{s,S}^t \right\} \quad (3.13)$$

where

$\rho_{s,p}$  = density of snowpack [kg m<sup>-3</sup>]

$\rho_1$  = constant, default value 200 kg m<sup>-3</sup>,

$\rho_2$  = constant, default value 0.5 m<sup>-1</sup>.

Knowing the density, an initial estimate of the depth of snow at the end of the time step,  $\Delta z_{s,est}^t$ , can be calculated as:

$$\Delta z_{s,est}^t = \frac{S_{s,S}^t}{f \cdot \rho_{w,p}^{t+\Delta t}} + P_s \cdot \Delta t \quad (3.14)$$

Based on this estimate, the final snow depth is calculated, considering the effect of water percolating through the snowpack:

$$\Delta z_s^{t+\Delta t} = \begin{cases} \frac{\Delta z_{s,est}^t \cdot S_{s,S}^{t+\Delta t}}{S_{s,S}^{t+\Delta t} - S_{w,Pond}^t + J_{w,S} \cdot \Delta t} & \text{if } J_{w,c} > S_{w,Pond}^t \\ \Delta z_{s,est}^t & \text{if } J_{w,c} \leq S_{w,Pond}^t \end{cases} \quad (3.15)$$

### 3.2.2 Canopy interception model

The amount of water present above the canopy will be rainfall ( $P_r$ ), overhead Irrigation water (e.g. sprinkler irrigation) ( $Irr^{OH}$  [mm h<sup>-1</sup>]), and meltwater, all of which is summarised in the expression  $J_{w,S}$ . This water may become throughfall, or, if intercepted, be evaporated, stored or flow to the ground as canopy spill-off.

The area covered by the crop is calculated as

$$A_C = 1 - \exp(K_I L_{ai}) \quad (3.16)$$

where



$K_I$  = empirical distribution coefficient, default 0.5 [-].

$L_{ai}$  = leaf area index [ $\text{m}^2 \text{m}^{-2}$ ].

### Throughfall

The direct through-fall is assumed to be a function of the leaf area index, and is estimated as:

$$J_{w,d} = J_{w,s}(1 - A_C) \quad (3.17)$$

where  $J_{w,d}$  is the direct through-fall [ $\text{mm h}^{-1}$ ].

The amount hitting the canopy will thus be:

$$Q_{C,in} = J_{w,s} \cdot A_C \quad (3.18)$$

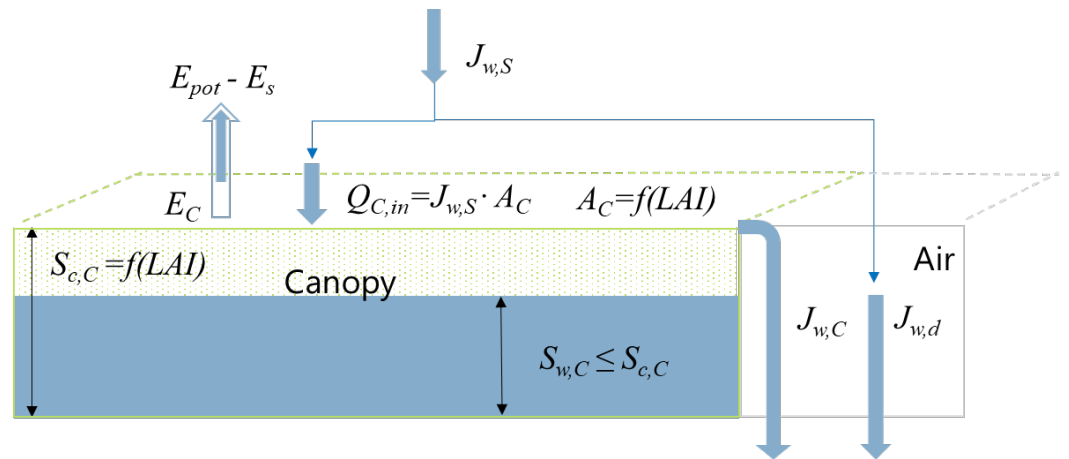


Figure 3.3. The major components of the water balance of the canopy compartment. Abbreviations used are described in the text below. The dotted lines illustrate that the canopy is an area, calculated as a function of LAI.

### Canopy storage capacity

The canopy storage capacity,  $S_{c,C}$  [mm] is assumed to be proportional to  $L_{ai}$ :

$$S_{c,C} = C_i L_{ai} \quad (3.19)$$

where  $C_i$  = interception capacity coefficient [mm], default 0.50 (Jensen, 1979).

### Evaporation from intercepted water

The potential canopy evapotranspiration ( $E_{p,C}$ ) [ $\text{mm h}^{-1}$ ] is calculated in two steps. First, the actual evaporation from the snow ( $E_s$ ) is deducted from the total potential evapotranspiration ( $E_p$ ). This amount is multiplied by the cover fraction ( $A_C$ ).

$$E_{p,C} = (E_p - E_s) \cdot A_C \quad (3.20)$$

The actual evapotranspiration from the canopy is equal to the potential if the amount of intercepted storage and incoming water can cover the demand. Otherwise, it is equal to the available water (incoming and stored):

$$E_C = \begin{cases} E_{p,C} & \text{if } (S_{w,S} > 0) \vee (Q_{in} > E_{p,C}) \\ Q_{in} & \text{if } (S_{w,S} = 0) \wedge (Q_{in} \leq E_{p,C}) \end{cases} \quad (3.21)$$

where

$E_C$  = the evaporation from the interception storage [ $\text{mm h}^{-1}$ ],

$S_{w,C}$  = the storage of intercepted water [mm], given by Eq. 3.23,

$E_{p,C}$  = the potential canopy evapotranspiration [ $\text{mm h}^{-1}$ ], given by Eq. 3.20.

### Canopy spill-off

The canopy spill-off is estimated as 0 as long as the rainfall minus actual evaporation does not make the storage overflow:

$$J_{w,C} = \begin{cases} 0 & \text{if } (Q_{C,in} \leq E_C) \vee (S_{w,C} < S_{c,C}) \\ (Q_{C,in} - E_C) & \text{if } (Q_{C,in} > E_C) \wedge (S_{w,C} = S_{c,C}) \end{cases} \quad (3.22)$$

where

$J_{w,C}$  = the flow to the ground as canopy spill-off [ $\text{mm h}^{-1}$ ]

and other variables are defined above. The value is negative because it leaves the canopy compartment.

### Canopy water storage

Finally, the canopy storage is updated considering the change within the timestep:

$$\frac{dS_{w,C}}{dt} = (Q_{C,in} - E_C - J_{w,C}) \quad (3.23)$$

$S_{w,C}$  and has values in the interval  $[0; S_{c,C}]$  due to the criteria specified in eq. 3.21 and 3.22.

#### 3.2.3 Litter layer

The default setting for the Litter layer is “none”, meaning that the effect of surface residuals is ignored by the model. There are, however, a standard litter model with two simple parameterisations (Maize and Millet) described here, and a more advanced mulch model described in appendix 3.1.

The amount of water reaching the litter layer is throughfall and canopy spill-off. In addition, water may be added through surface irrigation ( $Irr^{Surf}$ ). Furthermore, tillage may change properties of the soil and any water that is not room for in the soil ( $Q_{till}$ ) will be added to the litter layer for computational purposes. As tillage should not be carried out in saturated soil, this should be a rare occurrence.

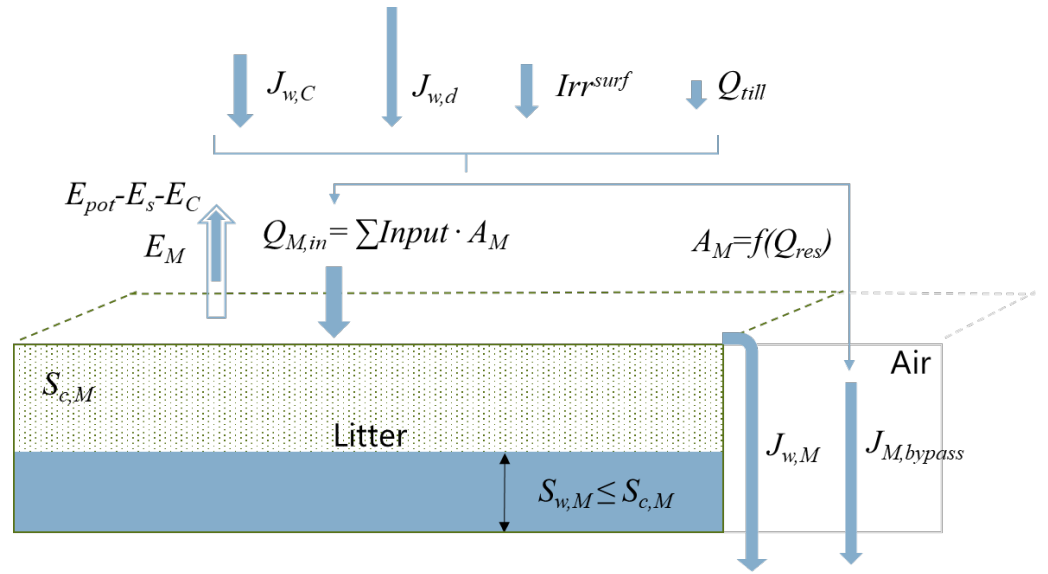


Figure 3.4. The major components of the water balance for the standard litter model. Abbreviations used are described in the text below. The dotted lines illustrate that mulch is treated as an area, calculated as a function of the mass of residue.

#### Litter interception

The amount of water intercepted by the litter ( $Q_{M,in}$ ) is the sum of the above mentioned inputs times the fraction of area with litter coverage,  $A_M$ .

$$Q_{M,in} = (J_{w,d} + J_{w,C} + Irr^{surf} + Q_{till}) A_M \quad (3.24)$$

$A_M$  is calculated from the amount of residue as:

$$A_M = 1 - \exp(-K_M Q_{res} Sp_{Mai}) \quad (3.25)$$

where

$Q_{res}$  = the amount of residue present [kg DM m<sup>-2</sup>],

$Sp_{Mai}$  = a specific AI describing the area covered by kg litter [m<sup>2</sup> cover/kg DM] and

$K_M$  = an extinction coefficient [-].

The last two parameters are specified for each of the parameterizations (Maize and Millet).

#### Litter bypass

The rest of the water arriving from above (not intercepted by the litter) is considered litter bypass.

$$J_{M,bypass} = (J_{w,d} + J_{w,C} + Irr^{surf} + Q_{till})(1 - A_M) \quad (3.26)$$

#### Litter storage capacity

The litter layer has a water storage capacity,  $S_{c,M}$  [mm], with different default values depending on the parameterization (Maize or Millet).

#### Evaporation from litter

The evaporation from water in the litter is calculated as

$$E_M = \begin{cases} E_{p,M} & \text{if } (S_{w,M} > 0) \vee (Q_{M,in} > E_{p,M}) \\ Q_{M,in} & \text{if } (S_{w,M} = 0) \wedge (Q_{M,in} \leq E_{p,M}) \end{cases} \quad (3.27)$$

Where  $S_{w,M}$  [mm] is the actual storage of water in litter, and

$$E_{p,M} = (E_{pot} - E_s - E_C) A_M \quad (3.28)$$

$E_{p,M}$  is thus the potential evapotranspiration from the litter layer [mm h<sup>-1</sup>].

#### Litter overflow

The overflow,  $J_{w,M}^{overflow}$  [mm h<sup>-1</sup>], is calculated as the amount of water that cannot be stored in the litter if there is water enough:

$$J_{w,M}^{overflow} = \begin{cases} 0 & \text{if } (Q_{M,in} \leq E_M) \vee (S_{w,M} < S_{c,M}) \\ (Q_{M,in} - E_M) & \text{if } (Q_{M,in} > E_M) \wedge (S_{w,M} = S_{c,M}) \end{cases} \quad (3.29)$$

#### Water stored in litter

Finally, the amount of water stored in litter is updated, considering the change within the timestep:

$$\frac{dS_{w,M}}{dt} = (Q_{M,in} - E_M - J_{w,M}^{overflow}) \quad (3.30)$$

$S_{w,M}$  has values in the interval  $[0; S_{c,M}]$  due to the criteria specified in eq. 3.28 and 3.29.

#### 3.2.4 Ponding and runoff

The water that is not stored in snow, canopy, or litter, or evaporated from those compartments, ends up at the soil surface,  $Q_{p, in}$  [mm h<sup>-1</sup>]. Ponding on the soil surface will occur if the water inputs (or storage from last time step) exceed the surface evaporation plus the soil infiltration. Infiltration simulated by the soil water model is described in Chapter 4. If no ponding occurs, infiltration is determined by the rate at which water is allocated to the surface. Calculations are done in two steps: first, the surface balance is calculated without considering infiltration into the soil, and second, the surface conditions define the upper boundary conditions for calculation of water infiltration in the soil.

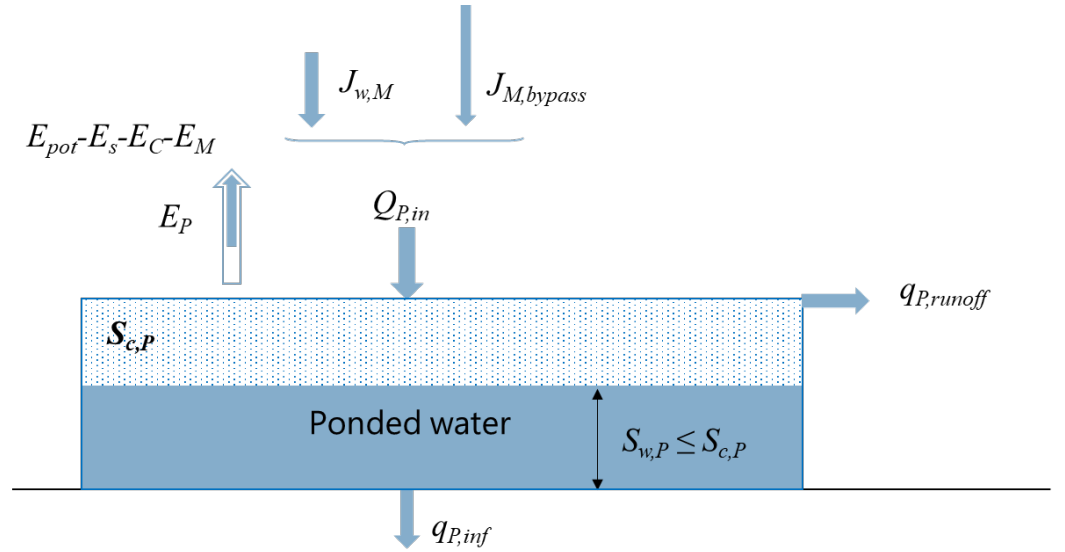


Figure 3.5. Major components of the water balance for water on the surface. Abbreviations are explained in the text below.

Evaporation from ponding water

The potential evaporation available for ponding,  $E_{p,Pond}$  [ $\text{mm h}^{-1}$ ], is:

$$E_{p,Pond} = (E_p - E_s - E_C)(1 - A_M) + (E_{P,M} - E_M) \cdot \gamma_M \quad (3.31)$$

describing that, for the area without litter, the total evaporation from free surfaces becomes equal to potential evaporation if water is available. For the litter-covered part of the surface, a vapour flux factor,  $\gamma_M$ , describes the reduction of the potential evapotranspiration below litter. It only affects the area covered by litter and has a default value of 0.

As long as water is available on the surface, it will evaporate at potential rate, so the actual pond evaporation ( $E_{Pond}$ ) will be the maximum of  $E_{p,Pond}$  and the available water.

Runoff

To mimic runoff, a runoff coefficient,  $k_{Pond}$  [ $\text{h}^{-1}$ ] can be specified, describing the fraction of the ponded water above the surface storage capacity that runs off each hour. Runoff is described as:

$$q_{runoff} = \max\{0; k_{Pond} (S_{w,Pond}^t - S_{c,Pond})\} \quad (3.32)$$

where

$q_{runoff}$  = the runoff rate [ $\text{mm h}^{-1}$ ]

$S_{w,Pond}^t$  = the ponding [mm], and

$S_{c,pond}$  = the surface storage capacity [mm], by default 1000 mm.

Ponding on soil surface

Finally, the amount of water stored on the soil surface as ponding is updated:

$$\frac{S_{w,Pond}}{dt} = Q_{Pond,in} - q_{runoff} - E_{Pond} - q_{Pond,inf} \quad (3.33)$$

Where  $E_{pond}$  [mm h<sup>-1</sup>] is the actual evaporation from ponded water and  $q_{Pond,inf}$  [mm h<sup>-1</sup>] is infiltration into the soil as a function of  $S_{w,P}$  and water flow in the soil described in chapter 4.

### 3.3 Soil evaporation and Transpiration

Calculation of actual evapotranspiration ( $E_a$ ) from the soil depends on the choice of “soil-vegetation-atmosphere-transfer” (SVAT) model selected. There are three SVAT models available in Daisy, the first of which is default and described here.

#### 3.3.1 SVAT-models

The available SVAT models are:

Decoupled surface energy and radiation (default)

1. A model in which the surface water balance and the surface energy and radiation balances are decoupled, which is the most commonly used version and described here. The upper boundary for the calculation of water movement and heat is described by the precipitation, air temperature and reference evapotranspiration (Hansen et al., 1990). The decoupled approach builds on the concepts of reference evapotranspiration and potential evapotranspiration. Here, potential evapotranspiration is the maximum evapotranspiration for a given vegetation. The potential evapotranspiration is related to the reference evapotranspiration by a simple crop coefficient (Hansen, 2002; Kjaersgaard et al., 2008),

Two-source by van der Keur et al.

2. A model in which the surface water balance and the surface energy and radiation balances are coupled, and evapotranspiration takes place from soil and canopy. This two-source model (soil and canopy) includes the stomata conductance stress function described by (van der Keur et al., 2001) which is influenced by solar radiation, temperature, vapour pressure, and soil moisture.

The SSOC-model

3. A model in which the surface water balance and the surface energy and radiation balances are coupled, and evapotranspiration takes place from soil as well as from shaded and sunlit leaves. This model includes a Ball-Berry type stomata conductance model (Ball et al., 1987; Plauborg et al., 2010), which is very detailed and requires information on leaf photosynthesis, and it takes into account chemical signalling (at present ABA) in the plant (Ahmadi et al., 2009). Leaf temperature, CO<sub>2</sub> concentration, and vapour pressure at leaf surfaces are state variables in this model. This module is referred to as the Sun-shade-open canopy (SSOC) module and is further described in Appendix 3.2 (not yet ready).

While the first approach can be used with daily data and even a simplified calculation of reference evapotranspiration not requiring humidity and wind

speed, the other two approaches, which are based on resistance/conductance theory require at least hourly values of precipitation, global radiation, temperature, wind speed and vapour pressure.

### 3.3.2 The uncoupled approach

Potential Evapotranspiration constitutes the upper limit for evapotranspiration in the standard SVAT model described here. If a more detailed description of surface conditions is required, one of the two more advanced SVAT models should be applied (van der Keur et al., 2001, Plauborg et al., 2010).

In the standard SVAT model, the potential evapotranspiration is a function of the crop growth through LAI and is calculated from the reference evapotranspiration as:

Potential surface evaporation and transpiration

$$E_{p,surf} = k_{crop} E_r^* \quad (3.34)$$

where

$$k_{crop} = \left( k_{c,soil} e^{-K_I L_{ai}} + k_{c,canopy} (1 - e^{-K_I L_{ai}}) \right) \quad (3.35)$$

or

$$k_{crop} = \left( k_{c,soil} (1 - A_C) + k_{c,canopy} A_C \right) \quad (3.36)$$

$E_{p,surf}$  = the potential evapotranspiration for soil evaporation and transpiration [mm h<sup>-1</sup> or mm day<sup>-1</sup>],

$k_{crop}$  = a crop coefficient [-], given by Eq. 3.35.

$k_{c,soil}$  = soil coefficient [-], by default 0.6, but may be user defined [*EpFactor*] and may be made a function of the pF-value of the top soil layer.

$k_{c,canopy}$  = canopy coefficient [-], by default 1.2 and

$E_r^*$  = the reference evapotranspiration in the same unit as  $E_p$ , corrected for evaporation from free surfaces ( $E_S + E_C + E_M + E_{Pond}$ ). This surplus amount is equal to ( $E_{p,Pond} - E_{Pond}$ ) and thus considers the effect of litter.

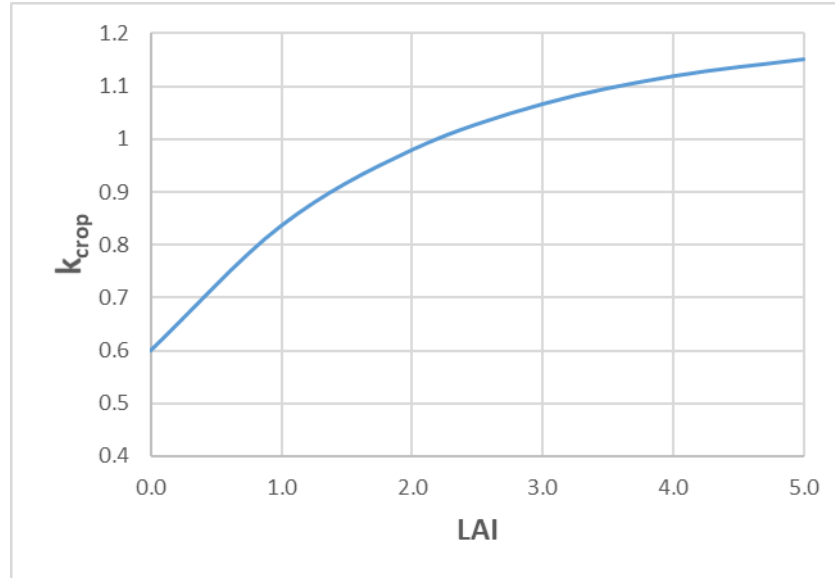


Figure 3.6. Relationship between  $k_{crop}$  and LAI with the default values for  $k_{c,soil}$  and  $k_{c,crop}$ .

In the presence of litter, part of the soil surface has a reduced evaporation potential or no evaporation, as  $\gamma_M$  by default is 0.

$$k_{crop} = \left( k_{c,soil} \left( (1 - A_C)(1 - A_M) + \gamma_M \cdot A_M \right) + k_{c,canopy} \cdot A_C \right) \quad (3.37)$$

#### Potential soil evaporation

The soil evaporation is assumed to be determined by either the energy which can be utilized by evaporation or the transport of soil water to the soil surface from beneath. The energy which can be utilized by soil evaporation is estimated as a fraction of the potential evapotranspiration (latent heat):

$$E_{p,soil} = k_{c,soil} \left( (1 - A_C)(1 - A_M) + \gamma_M \cdot A_M \right) \cdot f_{k,soil}(pF) \cdot E_r^*$$

where

$E_{p,soil}$  is the potential evaporation from soil surface [ $\text{mm h}^{-1}$ ] or [ $\text{mm d}^{-1}$ ] and

$f_{k,soil}$  [-] is a modifier-function that allows modification of  $k_{c,soil}$  as a function of water content expressed by pF.

The actual soil evaporation now depends on the rate at which soil water can be transported to the soil surface:

$$E_{soil} = \text{MIN} \left\{ E_{p,soil}; J_{w,Soil\_exf} \right\} \quad (3.38)$$

where

$E_{soil}$  = the actual soil evaporation [ $\text{mm h}^{-1}$ ] or [ $\text{mm d}^{-1}$ ], and

$J_{w,Soil\_exf}$  = a potential exfiltration rate [ $\text{mm h}^{-1}$ ], which is determined by the soil water model (see Chapter 4).



Potential transpiration

The potential transpiration is calculated as:

$$E_{p,t} = (E_{p,surf} - E_{p,soil}) + \beta(E_{p,soil} - E_{soil}) \quad (3.39)$$

where

$E_{p,t}$  = the potential transpiration [ $\text{mm h}^{-1}$ ], and

$\beta$  = a transfer coefficient allowing for the transfer of energy from a dry soil surface to the canopy (default value  $\beta = 0.6$  [-]). The actual transpiration is determined by the roots' ability to extract water from the rooting zone.

### 3.4 Heat transport in above-ground compartments

#### 3.4.1 Concepts

Equations in this section aim to describe the upper boundary conditions for the calculation of heat fluxes and temperatures in the soil for the default SVAT model (see the SSOC-model for another approach). These boundary conditions constitute a surface temperature and a temperature allocated to infiltrating water.

In the default SVAT model, the temperature of rain is given by the air temperature. If hourly air temperature values are available from the weather input file, these are used directly. If daily minimum and maximum temperatures are specified, the temperature is extrapolated over the day as described in Section 2.2.4. Water stored on leaves or mulch is assumed to obtain air temperature during storage. More complicated calculations are carried out for a snowpack and water standing on the surface (ponded water). The temperature of water fluxes depends on their origin and how different sources are mixed.

#### 3.4.2 Calculations

Water entering above snow and canopy

Liquid water entering from above may be rain or overhead irrigation. The temperature of the water hitting a snowpack,  $T_{top}$  [ $\text{mm hr}^{-1}$ ], or the compartments below (canopy, litter, soil surface) if a snowpack is not present, is calculated as:

$$T_{top} = (Irr^{OH} \cdot T_{Irr,OH} + P_r \cdot T_r) / (Irr^{OH} + P_r) \quad (3.40)$$

$Irr^{OH}$  = rate of overhead irrigation [ $\text{mm hr}^{-1}$ ]

$T_{Irr,OH}$  = Temperature of irrigation water [ $^{\circ}\text{C}$ ]

$P_r$  = rainfall as rain, [ $\text{mm hr}^{-1}$ ]

$T_r$  = max (air temperature, 0.1) [ $^{\circ}\text{C}$ ]

Heat calculations in snow

If snow is present and the snow contains liquid water, it is assumed that the surface temperature is  $0^{\circ}\text{C}$ . If snow is present and 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:

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

Or

$$T_{Surf} = \frac{(K_{h1}/z_1)T_1 + (K_s/\Delta z_s)T_a}{(K_{h1}/z_1) + (K_s/\Delta z_s)} \quad (3.41)$$

$T_{Surf}$  = surface temperature [K]

$T_a$  = air temperature [K]

$T_1$  = soil temperature at  $z_1$  [K]

$z_1$  = soil depth [m]

$\Delta z_s$  = depth of snow cover [m]

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

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

Melt water leaving the snowpack will have a temperature of 0 °C.

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

$$K_s = S\rho_s^2 \quad (3.42)$$

$S$  = empirical parameter [ $2.86 \cdot 10^{-6} W m^5 kg^{-2} K^{-1}$ ]

$\rho_s$  = density of snowpack [ $kg m^{-3}$ ] given by eq. 2.13 in chapter 3.

#### Heat in canopy

Water stored on the canopy is assumed to obtain the temperature  $T_r$  (=max (air temperature, 0.1) during storage, independent of its earlier temperature, while the temperature of water coming from above is either 0°C (if a snowpack is present) or calculated as Eq. 3.40. Similarly, the temperature of water below the canopy is calculated by multiplying the amount of canopy water bypass with either melt water temperature (if melt water is present) or with rain and (if present) irrigation temperatures, canopy drip off with canopy water temperature, surface irrigation water with the respective temperature and tillage water with rain temperature, adding the components and dividing by the total amount of water.

#### Heat in litter and pond

The same type of calculation is carried out for litter and input to ponded water. For litter/mulch, water stored in the litter/mulch is assumed to have obtained the temperature  $T_r$  (=max (air temperature, 0.1) during storage, similar to water stored on the canopy. Contrary to water stored on canopy or in litter, ponded water change temperature due to mixing with water from above. The mixing temperature is calculated:

$$T_{Pond}^{*t+\Delta t} = \frac{(T_{Pond}^t \cdot S_{w,Pond}^t + T_{in} \cdot Q_{Pond,in} \cdot \Delta t)}{(S_{w,Pond}^t + Q_{Pond,in} \cdot \Delta t)} \quad (3.43)$$

where

$T_{pond}$  = temperature of the ponded water [K]

$T_{in}$  = temperature of water coming into the pond [K]

Interactions with  
calculations of heat in  
the soil

From the calculations above, all infiltrating water (fluxes) have been allocated a temperature. In the presence of a snowpack or water standing on the surface (ponded water), the layer above the soil may have a temperature different from air temperature. In the case of a snowpack, the surface temperature is calculated as a function of air temperature and soil temperature, as shown in eq. 3.41. When no snow is present, the surface obtains the temperature of the layer above directly or over time. The temperature change from timestep to timestep may be dampened to stabilize the boundary condition for temperature calculations in the soil.

Changes depend on the setting of the parameter [*temperature\_change\_rate*]  $\zeta$  [[h<sup>-1</sup>],  $0 < \zeta < 1$ , default 0.5]. If this parameter is given a negative value, the temperature of the compartment above directly influences the surface temperature. If the parameter is set to a positive value, the surface temperature changes from one timestep to another are dampened. The change in a timestep is calculated as:

$$T_{Surf}^{t+\Delta t} = (T_{Surf}^{*t+\Delta t} - T_{Surf}^t) \cdot \min(\zeta * \Delta t, 1.0) \quad (3.44)$$

## 3.5 Solute transport in above-ground compartments

### 3.5.1 An overview

The objective of the solute balance model is to keep track of solutes allocated to, or released within, the system. Ammonium, nitrate, and pesticide balances are specialisations of the solute balance. The total solute balance comprises a solute balance for the above-ground processes described here and a soil solute balance described in Chapter 6.

Chemicals in Daisy cover descriptions of tracers, pesticides, and plant toxins as well as ammonium and nitrate. Chemicals can be added to the system from the top as dry and wet deposition, with a spray action, as a concentration in irrigation water, and/or as release from plants. The chemicals will then move down through the different surface compartments, if present, following the movement of above-ground water: The snowpack, canopy, litter, ponded water, and soil surface. At the soil surface solutes will infiltrate the soil either as matrix infiltration or

through cracks and biopores (see Chapter 6). Additionally, chemicals can sorb to and be moved with colloids generated at the soil surface (see Appendix 3.4).

This section focuses on the above-ground processes, but the soil surface is a transition zone, where soil processes may dominate. In the soil, transport, decomposition, sorption, diffusion, and crop uptake are major processes affecting solute fate. The decomposition can be influenced by temperature, water content, concentration of the compound and depth. Additionally, decomposition can have a lag-phase. A compound can break down into metabolites. Breakdown to metabolites is considered in the soil and can be, if specified, considered at the surface. Solute transport, sorption and sorption isotherms, sorption kinetics, and transformation in the soil is described in chapter 6 and processes specific for nitrogen and pesticides in the soil is described in chapter 7 and 8, respectively.

Dissipation and breakdown are treated as 1<sup>st</sup> order processes in Daisy. The change in solute content in a compartment is calculated based on the following equation, which is valid for all 1<sup>st</sup> order processes:

$$\begin{aligned} \frac{\partial S^t}{\partial t} &= I - S^t \cdot L \cdot \partial t \Rightarrow \\ S^t &= c_1 \cdot \exp(-L \cdot t) + I / L \end{aligned} \quad (3.45)$$

where

$c_1 = S^0 - I/L$ , and

$I$  = the absolute input rate,

$L$  = the relative loss rate and

$S^t$  = the storage at specific time ( $S^0$  = storage at  $t=0$ ).

In the case of several loss processes taking place at the same time,  $L$  in eq. (3.45) represents the sum of the individual loss rates. The total amount lost is then distributed between the breakdown processes according to the fractions that each breakdown rate constitutes of the sum of breakdown rates.

In the following description,  $S^C$  is used as notation for mass of chemical or solute in a compartment, while  $J^C$  is used for fluxes, parallel to the description of water. Figure 3.1 provides an overview of compartments and balances.

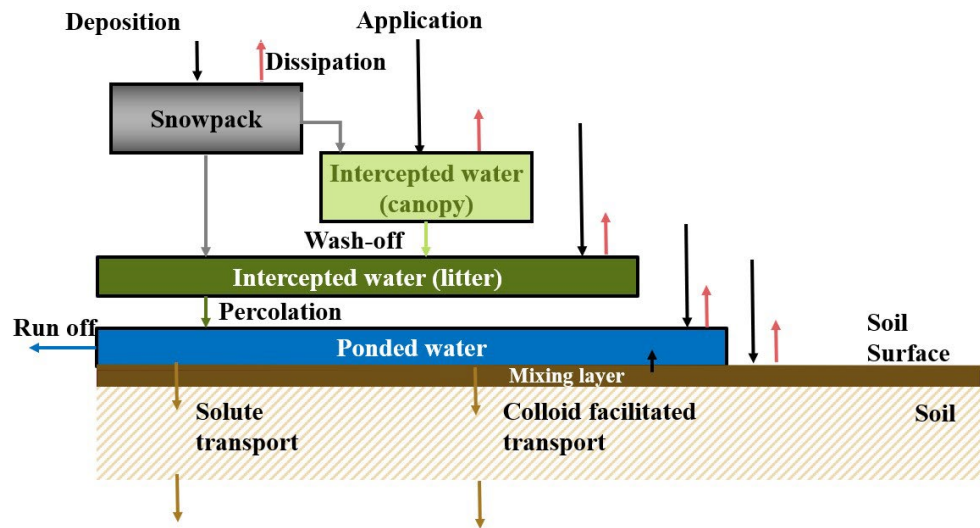


Figure 3.7. Schematic overview of solute transport processes at the surface.

### 3.5.2 Definition of a chemical

To function as a solute in Daisy, a chemical must be defined. Some examples are available under “lib” in the Daisy directory (see chemistry-base.dai and chemistry.dai). Depending on the chemical and the relevant processes different parameters can be defined. For the above-ground processes, the most important factors are solubility, canopy dissipation rate (or half-life) and canopy wash-off coefficient, litter decomposition rate (or half-life) and wash-off coefficient and surface decomposition rate (or half-life). The decomposition rate equals  $\ln(2)/\text{half-life}$ , so only one of the two should be defined. Initial contents of the compound in snow, on canopy, on litter and/or on the surface can also be specified. For the soil processes, decomposition, sorption, diffusion coefficient and the crop uptake reflection factor are the major parameters (see chapter 6). These can also define solute fate on the surface. If metabolites are included, the molar mass of the compounds and the fractions of the initial molecules becoming the metabolite must be specified.  $\text{CO}_2$ -production during breakdown can be specified.

A chemical can, to the largest extent possible, follow the parameterisation requirements used in [FOCUS](#) (pesticide guidelines). The main difference from the FOCUS approach is the description of wash-off from canopy, see Appendix 3.3.

Parameterisations and processes specific for pesticide are described in Chapter 7.

Ammonium and nitrate are pre-defined as “nutrients” with a canopy dissipation rate of 0 [ $\text{h}^{-1}$ ], a canopy wash-off coefficient of 1 and a decomposition rate of 0 [ $\text{h}^{-1}$ ]. Processes specifically defined for mineral nitrogen are described in Chapter 6.

### 3.5.3 Input of chemicals above the soil surface

Chemicals are typically added through deposition ( $\text{NO}_x$  and  $\text{NH}_3$ ), through spraying (e.g., pesticides), as fertilizer (see Chapters 7, 9 and 11) or with irrigation water (liquid fertilizers and perhaps other compounds, typically with drip irrigation).

|               |  |
|---------------|--|
| Deposition    | Deposition of ammonium and nitrate-N is specified in the Daisy weather file (see section 2.2.5). Dry deposition is specified as kg NH <sub>4</sub> -N ha <sup>-1</sup> year <sup>-1</sup> and kg NO <sub>3</sub> -N ha <sup>-1</sup> year <sup>-1</sup> [or kg m <sup>-2</sup> day <sup>-1</sup> ]. Wet deposition of the same two compounds is specified as a concentration, typically ppm [mg l <sup>-1</sup> ]. The rates should be calculated based on measurements. In Denmark, annual estimates are available from DCE (Institute for environmental science), Aarhus University. Concentrations for wet deposition in kg ha <sup>-1</sup> require re-calculation, considering the annual rainfall. |
| Spraying      | Spraying of a chemical (pesticide) is specified through the “spray” management operation. It requires an amount [g ha <sup>-1</sup> ] and information about timing and whether it is above or below the canopy (See Chapter 10 on management operations). In reality, spraying of e.g., pesticides will typically include water and solute. The amount of water allocated during pesticide spraying is typically around 200 L/ha or 0.02 mm, hence the amount of water applied during spraying is considered negligible. If larger amounts of water are applied with the solute, the operation can be defined as irrigation instead.   |
| Fertilization | Fertilizers including ammonium, nitrogen, urea, or organic manure can be added as a management operation (Chapter 10). For breakdown of plant materials and manure, see Chapter 8. Inorganic parts of the fertilizers are treated as solutes.  |
| Irrigation    | Solutes in irrigation water can be specified with a concentration and then applied when irrigating. Irrigation can take place as overhead irrigation (above canopy), as drip irrigation (at the surface) or as drip irrigation at a specified depth in the soil (Chapter 10).  |

#### 3.5.4 Solutes in snow

Input to snow,  $J_{S,in}^C$ , may come from overhead spray,  $J_{sprayOH}^C$ , deposition,  $J_{dep}^C$ , or overhead irrigation,  $J_{IrrOH}^C$ . Inputs are expressed as rates e.g. [g m<sup>-2</sup> hr<sup>-1</sup>], which is straight forward for spray and dry deposition. Wet deposition is calculated by multiplying the specified concentration in the precipitation with the rate of precipitation in the time step. Total input to the system, from above, is thus calculated as:

$$J_{S,in}^C = J_{sprayOH}^C + J_{dep}^C + J_{IrrOH}^C \quad (3.46)$$

Or

$$J_{S,in}^C = J_{sprayOH}^C + J_{drydep}^C + P \cdot c_{wetdep} + Irr_{OH} \cdot c_{IrrOH} \quad (3.47)$$

where  $c_{wetdep}$  [g m<sup>-2</sup> mm<sup>-1</sup>] and  $c_{IrrOH}$  [g m<sup>-2</sup> mm<sup>-1</sup>] are concentrations of solute in precipitation and overhead irrigation water, respectively.

Solutes in snow are, in Daisy, considered to be dissolved in the water within the snow compartment, and there is no dissipation.

Change in solute storage  
in snow

The change in solute content in the snow compartment is calculated based on eq. (3.45). In this case, the loss of solute is equal to outflow of solute as no other loss processes take place in the snow. For the snow compartment, the outflow of solute is proportional to the outflow of water (see section 3.2.1). Thus, the relative loss rate is defined as

$$k_{S,loss}^C = \frac{J_{w,S}}{S_{w,S}^{t+\Delta t} + J_{w,S} \cdot \Delta t} \quad (3.48)$$

where  $k_{S,loss}^C$  has the unit [ $h^{-1}$ ] and is represented by L in eq. (3.45).

Outflow of solute

The total loss of solute from the snowpack is then calculated as:

$$J_{w,S}^C = S_S^{C,t} - S_S^{C,t+\Delta t} + k_{S,loss}^C \cdot \Delta t \quad (3.49)$$

where  $J_{w,S}^C$  [ $g\ m^{-2}\ h^{-1}$ ] equals the outflow of solute with water from the snowpack and  $S_S^C$  [ $g\ m^{-2}$ ] equals storage of chemical in the snow. Solute leaving the snow compartment,  $J_{w,S}^C$ , follows the water to “the top of the canopy”. If there is no snow,  $J_{w,S}^C$  will equal  $J_{S,in}^C$  given by eq. (3.46)/(3.47).

### 3.5.5 Solute on canopy

Solutes arriving at the top of the canopy may be caught on the leaves or continue as through-fall. Through-fall is assumed to be a function of the leaf area index and is estimated as:

$$J_{w,d}^C = J_{w,S}^C (1 - A_C) \quad (3.50)$$

where  $A_C$  stem from eq. (3.16) and  $J_{w,d}^C$  is the solute in the through-fall [ $g\ m^{-2}\ hr^{-1}$ ]. The rest of the solute is intercepted by the canopy, where it may dissipate, be stored, or be washed off.

Input to canopy

The absolute input rate to the canopy,  $Q_{C,in}^C$  [ $g\ m^{-2}\ h^{-1}$ ], at a given time is the amount received from above plus any contribution (positive or negative) from degradation of products already on the canopy ( $R_{C,transform}^C$ ) minus solute lost with plant material being harvested ( $J_{C,harvest}^C$ ) or dropped from the plant as residuals ( $J_{C,residual}^C$ ).

$$Q_{C,in}^C = (J_{w,S}^C \cdot A_C) - J_{C,harvest}^C - J_{C,residuals}^C + R_{C,transform}^C \quad (3.51)$$

Losses from canopy

The relative loss rate from the canopy is the sum of the canopy wash-off rate, [ $h^{-1}$ ],  $k_{w,C}^C$  and the canopy dissipation rate,  $k_{C,diss}^C$  [ $h^{-1}$ ].

The canopy wash-off rate is calculated as the canopy wash-off coefficient,  $\kappa_{w,C}^C$  [ ] multiplied by the relative canopy spill-off ( $J_{w,C}$ , eq.(3.22)) at a given time.

$$k_{w,C}^C = \kappa_{w,C}^C \cdot \frac{J_{w,C}^C}{S_{w,C}^t} \quad (3.52)$$

The canopy dissipation rate  $k_{C,diss}^C$  mimics the effects of uptake in the leaves and all loss processes on the leaves (e.g., photolysis, volatilization). It is specified by the user.

The new storage on the canopy ( $S_{w,C}^{C,t}$ , [g m<sup>-2</sup>]) is calculated according to eq. (3.45), where L represents the sum of the wash-off rate and the dissipation rate. The combined total loss ( $LOSS_{canopy}$ ) from wash-off ( $J_{w,C}^C$  [g m<sup>-2</sup> h<sup>-1</sup>]) and dissipation ( $R_{C,diss}^C$  [g m<sup>-2</sup> h<sup>-1</sup>]) is calculated similarly to eq. (3.49) for the snow compartment. The loss from the canopy is divided between the two loss processes according to the fraction of the total loss rate made up by each of them.

$$J_{w,C}^C = LOSS_{canopy} \frac{k_{w,C}^C}{k_{w,C}^C + k_{diss,C}^C}$$

$$R_{diss,C}^C = LOSS_{canopy} \frac{k_{diss,C}^C}{k_{w,C}^C + k_{diss,C}^C} \quad (3.53)$$

The total amount of solute moving to the next compartment from the canopy is the solute in canopy wash-off plus the loss of solute with residuals.

### 3.5.6 Solute in litter

#### Input to litter

The total amount of solute available above a litter layer ( $Q_{M,in}^C$  [g m<sup>-2</sup> h<sup>-1</sup>]) is the amount lost from the canopy itself (eq. (3.53) above), the canopy throughfall and any solute sprayed or distributed with irrigation water on the litter (i.e. below the canopy), plus any contribution from degradation of products already on the litter. The addition of solute to the litter at a given time will then be:

$$Q_{M,in}^C = (J_{w,C}^C + J_{w,d}^C + Irr_{surf} \cdot c_{irr\_surf}) \cdot A_M + J_{C,residuals}^C + R_{M,transform}^C \quad (3.54)$$

Where

$Irr_{surf}$  = surface irrigation [mm hr<sup>-1</sup>]

$c_{irr\_surf}$  = concentration of solute in surface irrigation water [g m<sup>-2</sup> mm<sup>-1</sup>]

$A_M$  = fraction of the surface covered by mulch [], and

$R_{M,transform}^C$  = contribution from degradation products on the mulch, [g m<sup>-2</sup> h<sup>-1</sup>]

The rest of the available solute is considered bypass ( $J_{M,bypass}^C$ ) calculated as:

$$J_{M,bypass}^C = (J_{w,C}^C + J_{w,d}^C + Irr_{surf} \cdot c_{irr\_surf}) \cdot (1 - A_M) \quad (3.55)$$

#### Losses from litter



Solute on the litter may be lost through wash-off or degradation. Additionally, solute in the alternative mulch model can diffuse from stored water to moving water (see Appendix 3.1). The wash-off rate from litter,  $k_{w,M}^C$  [h<sup>-1</sup>] is calculated similarly to the wash-off from canopy, based on a wash-off coefficient,  $\kappa_{w,M}^C$  [], and the rate of water leaching from the litter, eq. (3.52):

$$k_{w,M}^C = \kappa_{w,M}^C \cdot \frac{J_{w,M}^t}{S_{w,M}^t} \quad (3.56)$$

Decomposition is specified either by a litter decomposition rate,  $k_{M,deg}^C$  [h<sup>-1</sup>] or as half-life [h]. The total relative loss rate from the canopy is then calculated as the sum of wash-off rate and decomposition rate.

The new storage in the mulch layer ( $S_{w,M}^{C,t}$ , [g m<sup>-2</sup>]) is calculated with Eq. (3.45) and the combined loss from spill-off ( $J_{w,M}^C$  [g m<sup>-2</sup> h<sup>-1</sup>]), and degradation ( $R_{M,deg}^C$  [g m<sup>-2</sup> hr<sup>-1</sup>]) is calculated similarly to eq. 3.49 for loss of solute from the snow compartment. The individual losses are calculated similarly to eq. (3.53).

### 3.5.7 Solute on the surface

Input to surface or ponded water

The solute passing by the litter layer or present in wash-off from the litter layer will continue to ponding water on the soil surface or the surface itself. If the mulch module (appendix 3.3) is activated, diffusion of solute ( $J_{w,M\_diff}^C$  [g m<sup>-2</sup> h<sup>-1</sup>]) also becomes an input. In addition, solute may be formed on the surface from decomposition of another compound ( $R_{Sf,transform}^C$  [g m<sup>-2</sup> h<sup>-1</sup>]) or exfiltrate from the soil to the surface ( $J_{w,Soil\_exf}^C$ ).

$$Q_{sf,in}^C = J_{M,bypass}^C + J_{w,M}^C + J_{w,M\_diff}^C + R_{Sf,transform}^C + J_{w,Soil\_exf}^C \quad (3.57)$$

The surface constitutes the boundary between above-ground and the soil, and to bridge this boundary, a mixing layer is introduced [default: 0.1 [cm]]. The mixing layer affects the exchange of solutes between soil water and water on the surface, and soil colloids, if present, especially under intense rainfall events. The water available at the surface is thus ponded water plus the soil water in the mixing layer. The mass of solute available is the mass of solute in the ponded water plus the mass stored in the mixing layer (sorbed and dissolved). The amount of soil available in the mixing layer is calculated based on the bulk density of the mixing layer, which will be equal to that of the topsoil. Sorption to the soil is then determined based on the sorption isotherm and parameters specified (see Chapter 6). The concentration of the water on the surface (ponded and in the mixing layer) of dissolved solute can then be determined.

Solutes in the soil can exfiltrate to the surface water (ponded and in mixing layer) if the concentration in the soil water is higher than the concentration in the surface water. The exfiltration is calculated based on the difference in

concentration on the surface (storage concentration) and in the topsoil (default the top 0.1 cm). The exfiltration can be delayed, using a resistance factor  $R_{mix}$  [default  $1 \cdot 10^9$ , h mm<sup>-1</sup>], so that the maximum amount that can exfiltrate to the surface water is  $(storage\ concentration - soil\ concentration) / R_{mix}$ .

#### Losses on the surface

Solutes may be lost with surface runoff, with water infiltrating the soil or due to decomposition. Infiltrating water has the calculated dissolved solute concentration. The rate of removal of solute with surface runoff is equal to the rate of loss of water,  $q_{runoff}$  calculated in eq. (3.32):

$$k_{runoff}^C = \frac{q_{runoff}}{S_{w,P}^t} \quad (3.58)$$

The decomposition factor for the solute on the surface and in ponded water (e.g., both sorbed and in solution),  $k_{sf,deg}^C$ , is specified as a decomposition rate or half-time of the surface. If the surface decomposition factor is not specified, the canopy dissipation rate is used, as it is assumed that the breakdown process dominating at the canopy also dominates at the soil surface. However, it can also be assumed that the breakdown process dominating in the soil also dominates at the soil surface. Thus, the decomposition factor for the soil can be used as the surface decomposition factor. In that case, the “*soil\_affects\_surface\_decompose*” should be activated, making the actual decomposition rate at the soil surface a function of water content and temperature in the mixing layer, as for decomposition in the soil (chapter 6). Similarly, if it is assumed that the breakdown process at the soil surface generates metabolites (as in the soil, see chapter 6) “*enable\_surface\_products*” should be activated. By default, both “*soil\_affects\_surface\_decompose*” and “*enable\_surface\_products*” are FALSE.

The new storage on the surface ( $S_{w,sf}^{C,t}$ , [g m<sup>-2</sup>]) is calculated with Eq. (3.45) and the combined loss to runoff ( $q_{p,runoff}^C$  [g m<sup>-2</sup> h<sup>-1</sup>]) and degradation ( $R_{sf,deg}^C$  [g m<sup>-2</sup> h<sup>-1</sup>]) is calculated similarly to eq. (3.49) for the snow compartment. The individual losses are calculated similarly to eq. (3.53) for the canopy.

Infiltration to the soil,  $J_{w,inf}^C$  [g m<sup>-2</sup> h<sup>-1</sup>], is then calculated as a function of the dissolved solute concentration in the surface water (ponded and in mixing layer) and amount of infiltration water,  $q_{pond,inf}$ , (described in chapter 4).

### 3.6 Parameter overview

Table 3.1. Related Parameter names in Daisy.

| Name and explanation                    |   | Model (in Daisy) | Parameter name<br>(Daisy reference manual) | Default                          | Default unit   |
|---|---|------------------|--|----------------------------------|--|
| <b><i>P</i></b>                         | Precipitation   | weather          | <i>Precip</i>                              | User input (hourly or daily)     | [mm h <sup>-1</sup> ]  |
| <b><i>E<sub>r</sub></i></b>             | Reference evapotranspiration  | weather          | <i>RefEvap</i>                             | Optional input (hourly or daily) | [mm h <sup>-1</sup> ]  |
| <b><i>Irr<sup>OH</sup></i></b>          | Addition of water with overhead irrigation                                  | Irrigation       | <i>flux</i>                                | User defined                     | [mm h <sup>-1</sup> ]  |
| <b><i>m<sub>f</sub></i></b>             | Snowpack depth melting factor   | Snow             | <i>mf</i>                                  | 10                               | [m <sup>-1</sup> ]   |
| <b><i>m<sub>i</sub><sup>*</sup></i></b> | Air temperature melting factor  | Snow             | <i>mtprime</i>                             | 0.0833333<br>(or 2.0)            | [kg m <sup>-2</sup> °C <sup>-1</sup> ·h <sup>-1</sup> ]<br>[kg m <sup>-2</sup> °C <sup>-1</sup> ·day <sup>-1</sup> ] |
| <b><i>m<sub>r</sub><sup>*</sup></i></b> | Radiation melting factor, eq. 3.9.  | Snow             | <i>mrprime</i>                             | 1.5·10 <sup>-7</sup>             | [kg J <sup>-1</sup> ]  |
| <b><i>m<sub>1</sub></i></b>             | Linear constant, eq. 3.9.   | Snow             | <i>m1</i>                                  | 2                                | []   |
| <b><i>m<sub>2</sub></i></b>             | Exponential constant, eq. 3.9.  | Snow             | <i>m2</i>                                  | 0.00416667                       | [h <sup>-1</sup> ]   |
| <b><i>ρ<sub>s</sub></i></b>             | Density of snow, eq. 3.8.   | Snow             | <i>rho_s</i>                               | 100                              | [kg m <sup>-3</sup> ]  |
| <b><i>f<sub>c</sub></i></b>             | Water capacity coefficient for retention of liquid water in snow, eq. 3.11. | Snow             | <i>f_c</i>                                 | 0.07                             | []   |
| <b><i>ρ<sub>1</sub></i></b>             | Water collapse factor, eq. 3.13.  | Snow             | <i>rho_1</i>                               | 200                              | [kg m <sup>-3</sup> ]  |

| <b>Name and explanation</b>   | <b>Model (in Daisy)</b> | <b>Parameter name<br/>(Daisy reference manual)</b> | <b>Default</b>                             | <b>Default unit</b>                   |
|---|-------------------------|--|--|---------------------------------------|
| $\rho_2$ Snow collapse factor, eq. 3.13.  | Snow                    | <i>rho_2</i>                                       | 0.5  | [m <sup>-1</sup> ]                    |
| $Psa$ Minimum amount of snow required for snow to become new.                   | Snow                    | <i>Psa</i>   | 5  | [mm day <sup>-1</sup> ]               |
| $fsa$ Relative amount of snow in precipitation required for snow to become new. | Snow                    | <i>fsa</i>   | 0.9  | []                                    |
| $K_I$ Empirical distribution coefficient, eq. 3.16.                             | CanopyStandard          | <i>EpExt</i>                                       | 0.5  | []                                    |
| $C_i$ Canopy interception capacity.   | CanopyStandard          | <i>IntepCap</i>                                    | 0.5  | [mm]                                  |
| $Irr^{Surf}$ Addition of water with surface irrigation.                         | Irrigation              | <i>flux</i>  | User defined                               | [mm h <sup>-1</sup> ]                 |
| $Sp_{Mai}$ Specific residue area index, eq. 3.35.                               | Litter/residue          | <i>specific_AI</i>                                 | depends on submodel (Maize, Millet, mulch) | [m <sup>2</sup> kg DM <sup>-1</sup> ] |
| $K_M$ Beer's law extinction coefficient for litter/mulch.                       | Litter/residue          | <i>extinction_coefficient</i>                      | depends on submodel (Maize, Millet, mulch) | []                                    |
| $S_{c,M}$ Water holding capacity of surface residuals.                          | Litter/residue          | <i>water_capacity</i>                              | depends on submodel (Maize, Millet, mulch) | [L kg DM <sup>-1</sup> ]              |
| $\gamma_M$ Reduction factor for potential evaporation below litter/mulch.       | Litter/residue          | <i>vapour_flux_factor</i>                          | default: 0, otherwise user specified.      | []                                    |

| Name and explanation |  | Model (in Daisy) | Parameter name<br>(Daisy reference manual) | Default                                      | Default unit                           |
|----------------------|--|------------------|--|--|--|
| $K_{soil}$           | Saturated hydraulic conductivity of the topsoil.   | hydraulic        | $K_{sat}$                                  | user defined (or from pedotransfer-function) | [cm h <sup>-1</sup> ]                  |
| $S_{c,P}$            | Maximum storage capacity on the soil surface.  | surface          | $DetentionCapacity$                        | 1000   | [mm]                                   |
| $k_P$                | Runoff coefficient. Fraction of ponding above maximum storage capacity that runs off every hour. | surface          | $ReservoirConstant$                        | 1  | [h <sup>-1</sup> ]                     |
| $k_{c,soil}$         | Conversion of $E_r$ to $E_p$ for bare soil.  | surface          | $EpFactor$                                 | 0.6  | []                                     |
| $f_{k,soil}(pF)$     | Modifier function of $k_{c,soil}$ as function of pF.   | surface          | $EpFactor\_SWE$                            | (0 1) (1 1)                                  | [pF []]                                |
| $k_{c,canopy}$       | Conversion of $E_r$ to $E_p$ for canopy.   | Canopy standard  | $EpFac$                                    | 1.2  | []                                     |
| $\beta$              | Redistribution of $E_p$ between transpiration and soil evaporation, eq. 3.39.                    | vegetation       | $EpInterchange$                            | 0.6  | []                                     |
| $f_{Ep,soil}(h)$     | modifier function for $f_{Ep,soil}$  | surface          | $EpFactor\_SWE$                            | (0 1) [1 1)                                  | [pF -> <none>[]]                       |
|                      | Dampens temperature changes at the soil surface  | surface          | $temperature\_change\_rate$                | 0.5  | [h <sup>-1</sup> ]                     |
| $T_{Irr,OH}$         | Temperature of irrigation water  | irrigation       | $temperature$                              | air temperature                              | [°C]                                   |
| $C_{irrOH}$          | concentration of solute in overhead irrigation water   | irrigation       | <i>specified with name and value</i>       | user specified                               | [g cm <sup>-2</sup> mm <sup>-1</sup> ] |

| Name and explanation  | Model (in Daisy) | Parameter name<br>(Daisy reference manual)                             | Default                          | Default unit                           |
|---|------------------|--|----------------------------------|--|
| $K_{w,C}^C$ canopy wash-off coefficient eq. 3.52.                               | chemical         | <i>canopy_washoff_coefficient</i>                                      | user specified                   | []                                     |
| $k_{C,diss}^C$ canopy dissipation rate  | chemical         | <i>canopy_dissipation_rate</i> ,<br><i>canopy_dissipation_halftime</i> | user specified                   | [h <sup>-1</sup> ]<br>[h]              |
| $C_{irr\_surf}$ concentration of solute in surface irrigation water             | irrigation       | <i>specified with name and value</i>                                   | user specified                   | [g cm <sup>-2</sup> mm <sup>-1</sup> ] |
| $K_{w,M}^C$ litter wash-off coefficient, eq. 1.77                               | chemical         | <i>litter_washoff_coefficient</i>                                      | user specified                   | []                                     |
| $k_{M,deg}^C$ Decomposition or degradation rate for solute on litter            | chemical         | <i>litter_decompose_rate</i><br><i>litter_decompose_halftime</i>       | user specified                   | [h <sup>-1</sup> ]<br>[h]              |
| $k_{Sf,deg}^C$ Decomposition or degradation rate for solute on the soil surface | chemical         | <i>surface_decompose_rate</i><br><i>surface_decompose_halftime</i>     | decomposition rate for the soil. | [h <sup>-1</sup> ]<br>[h]              |
| If decomposition at the surface is affected by soil factors.                    | chemical         | <i>soil_affects_surface_decompose</i>                                  | FALSE                            | [-]                                    |
| If decomposition at the surface generate metabolites.                           | chemical         | <i>Enable_surface_products</i>   | FALSE                            |  |
| $R_{mix}$ Resistance to exfiltration from soil to surface.                      | surface          | <i>R_mixing</i>  | 1e+09                            | [h mm <sup>-1</sup> ]                  |

|                          |            |                   |
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| Styczen, M. & Holbak, M. | 2023 06 13 | 6.23              |

### 3.7 Appendices

3.1: The mulch model.

3.2: The Sun Shade Open Canopy (SSOC)-SVAT model (not prepared).

3.3: Alignment of Daisy with FOCUS recommendations.

3.4: Colloid generation.

### 3.8 References

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