

Equation Section 1

Daisy, a flexible Soil-Plant-Atmosphere system Model

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SUMMARY.

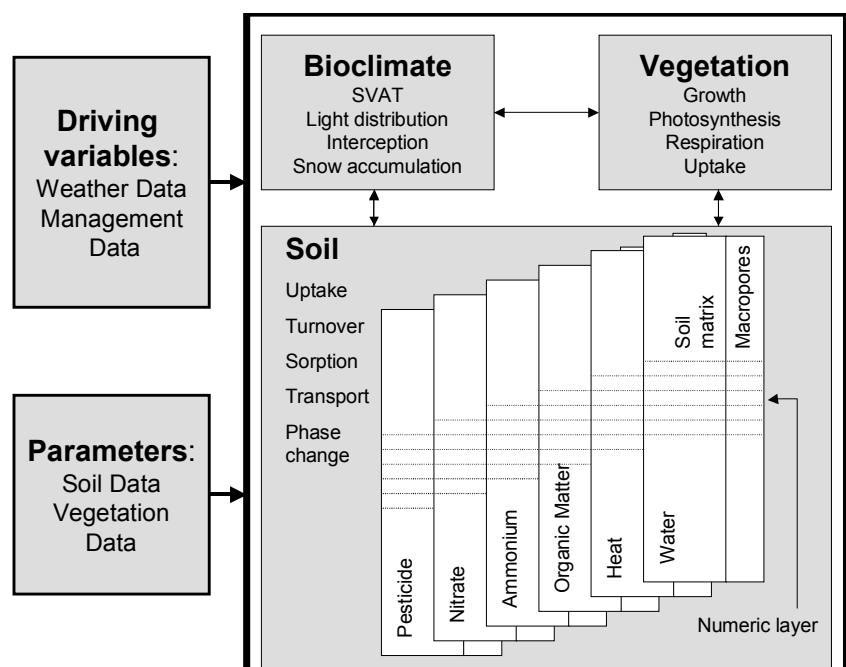
Daisy is a Soil-Plant-Atmosphere system model designed to simulate water balance, heat balance, solute balance and crop production in agro-ecosystems subjected to various management strategies. The water balance model comprises a surface water balance and a soil water balance. The surface water includes a model for snow accumulation and melting, a model for interception, through-fall, and evaporation of water in the crop canopy, and a model for infiltration and surface run-off. The soil water balance includes water flow in the soil matrix as well as in macropores. Furthermore, it includes water uptake by plants and a model drainage to pipe drain. The heat balance model simulates soil temperature and freezing and melting in the soil. The solute balance model simulates transport, sorption and transformation processes. Special emphasis is put on nitrogen dynamics in agro-ecosystems. Mineralization-immobilization, nitrification and denitrification, sorption of ammonium, uptake of nitrate and ammonium, and leaching of nitrate and ammonium are simulated. Degradation, sorption, uptake and transport of agro-chemicals like pesticides are simulated. The crop production model simulates plant growth and development, including the accumulation of dry matter and nitrogen in different plant parts. Furthermore, the development of leaf area index and the distribution of root density are simulated. Competition for light, water and nitrogen between plant species are also simulated. The agricultural management model allows for building complex management scenarios. The model can work distributed with multiple soil columns. A facility to link the model to hydrological catchment models exists. This facility has been applied to link Daisy to the distributed hydrological catchment model MIKE/SHE. Furthermore, the very flexible Daisy software allows for implementation of different process descriptions of the same process. The selected process description is chosen by the model parameterization.

INTRODUCTION

The loss of agrochemicals into aquifers and surface waters in humid regions is an inevitable consequence of intensive agriculture. In large parts of Europe, for instance, the input of nitrogen to agricultural systems and subsequent losses are so large that they constitute a threat to both the quality of surface and ground waters (EEA, 1995). In most agricultural systems the main loss of nitrogen is due to leaching of nitrate from the fields. The fact that laboratory and field measurements necessary for assessment of nitrogen leaching from agricultural fields are expensive have prompted the development of agro-ecosystem models capable of simulating the nitrogen dynamics in agricultural soils and in particular simulating the leaching. In Denmark this led to the development of the Daisy model (Hansen *et al.*, 1990, 1991a). This model has since then been used extensively (e.g. Blicher-Mathiesen *et al.*, 1990; Blicher-Mathiesen *et al.*, 1991; Hansen *et al.*, 1991b; Hansen *et al.*, 1992; Hansen and Svendsen, 1994, 1995a,b,c; Hansen *et al.*, 1999, Jensen and Østergaard, 1993; Jensen *et al.*, 1992; Jensen *et al.*, 1993; Jensen *et al.*, 1994a,b; Jensen *et al.*, 1996; Magid and Kølster, 1995; Mueller *et al.*, 1997; Petersen *et al.*, 1995; Refsgaard *et al.*, 1999, Styczen and Storm, 1993a,b). The model applications comprise both scientific studies and management related studies aimed at decision support. In addition, the model has been validated in a number of major comparative tests (Vereecken *et al.*, 1991; Hansen *et al.*, 1991a,c; Willigen, 1991; Diekkrüger *et al.*, 1995; Svendsen *et al.*, 1995; Smith *et al.*, 1997; Jensen *et al.*, 1997). Hence, Daisy can be considered a well-tested model.

Daisy is a one-dimensional agro-ecosystem model that, in brief, simulates crop growth, water and heat balances, organic matter balance, the dynamics of ammonium and nitrate in agricultural soil based on information on management practices and weather data, Fig. 1. Recently, the simulation of the fate of pesticides has been included in the model. The simulation of the organic matter balance and the nitrogen dynamics is strongly interconnected, hence the organic matter model is considered an integral part of the overall nitrogen balance model. Weather data are used as driving variables. The minimum data requirement is daily values of global radiation, air temperature and precipitation. However, much more detailed information can be utilized by the model, e.g. hourly values of global radiation, air temperature, relative humidity, wind speed, and precipitation. The present chapter offers a relatively detailed description of the Daisy model.

Figure 1. Schematic representation of the agro-ecosystem model Daisy. The model comprises three main modules, viz. a bioclimate, a vegetation, and a soil component.



THE DAISY MODEL SOFTWARE

The experience obtained with the original implementation of the Daisy model called for an extension of the functionality of the model software. In scientific studies, a wish often exists for testing alternative process model formulations and for adding new process models. An example of the former would be a study of the nitrification process where alternate process descriptions would be tested. An example of the latter would be a study of pesticide fate in soil. Furthermore, in management oriented studies, the ability of the model to make use of alternate process-description makes it possible to choose the process-description on the basis of the required accuracy, the available data or available resources in terms of computer-time. In simulation studies of organic farming systems a distinct need for the ability to simulate inter-cropping systems was recognized. In environmental impact assessment related studies, e.g. studies on groundwater quality, it was recognized that an implementation that supports the linkage at code level of Daisy with other model systems would be very beneficial. E.g. Styczen and Storm (1993a,b) linked Daisy with a fully distributed catchment model, MIKE SHE (Abbott *et al.*, 1986) in order to simulate groundwater quality within a hydrological catchment. However, in order to do this they had to run the two components of the combined model system MIKE SHE /Daisy iteratively. Such a procedure is sub-optimal.

In order to comply with the needs and wishes indicated in the above section, the Daisy model software has been reimplemented within the framework of the Danish Informatics Network in Agricultural Sciences. The new model software offers extensions as compared with the original implementation while the old functionality is maintained. The new model software supports:

- simulation of multiple soil columns, which make distributed modelling possible.
- linkage to other computer models (an interface to MIKE SHE has been developed).
- simulation of inter-cropping systems.
- selection among alternative process-description (e.g. water flow in the unsaturated zone, soil hydraulic parameter models).
- introduction of new process-models (e.g. macropore flow, degradation and sorption of agrochemicals (pesticides)).

The new implementation has developed the model into an open software system, the principles of which are described by Abrahamsen and Hansen (2000).

Initialization and parameterization of Daisy is done in a special setup file, which is read by a special parser component. The input system is very flexible, it allows for storing full or partial parameterizations of selected process models in separate library files. The information stored in the library file is included in the set-up by a simple reference to the library file (Abrahamsen and Hansen, 2000). E.g., this facility is used for storing crop parameterizations in a crop library, and by including the crop library or crop libraries the various crop parameterizations are available just by referring to the name under which the parameterization is stored. Similarly, soil information required to parameterize a soil horizon can be stored in a soil horizon library and referred to by name.

If more than one process model description is implemented, the selection between these implementations is done in the parameterization. Furthermore, the parser allows for the allocation of default values to model parameters. This facility is applied to allocate default values to model parameters whenever it is feasible. Parameters, which are not given a specific value, need not

appear in the input files.

The output system is also very flexible and allows the user to define his own output, which can be very detailed or only contain major simulation results. Output files are readily read by common spreadsheet software.

WATER BALANCE

The water balance component of the model deals with the water balance of the surface and the soil. Hence the atmosphere and the ground water constitute the boundaries of the considered system. Considered fluxes at the surface are precipitation and irrigation (gains), and evapotranspiration and surface runoff (losses). Considered fluxes at the lower boundary of the system are deep percolation (loss) or capillary rise (gain) and if the considered system contains artificial drain also drain flow (loss).

The modeling of surface fluxes of water is especially complicated as it also involves exchange of energy fluxes. In Daisy this problem is coped with by introducing the concept of potential evapotranspiration (PET). PET acts as the driving force in evapotranspiration modeling and constitutes the upper limit for evapotranspiration. If a more detailed description of surface conditions is required, Daisy also includes the soil-vegetation-atmosphere transfer model based on a resistance network (Shuttleworth and Wallace, 1985; Shuttleworth and Gurney, 1990; Keur *et al.* 2000). The latter model requires detailed weather data, i.e. hourly values of weather data measured at the considered site.

Potential Evapotranspiration

PET can be obtained in different ways: i) it can be supplied to the model together with other “weather data”; ii) it can be based on a reference evapotranspiration based on the Penman-Montheith formula as recommended by FAO (1990); or iii) it can be based on reference evapotranspiration calculated by a simple empirical equation, viz the Makkink equation (Makkink, 1957; Hansen, 1984). The potential evapotranspiration is calculated from the reference evapotranspiration by the relation:

$$E_p = C_c E_r \quad (1.1)$$

where E_p is the potential evapotranspiration, C_c is a crop factor (default value $C_c=1.0$), and E_r is the reference evapotranspiration.

The FAO reference evapotranspiration for short grass is calculated from the Penman-Montheith formula:

$$E_r = \frac{\Delta(R_n - G) + \rho c_p (e_s - e_a) / r_a}{\lambda (\Delta + \gamma (1 + r_c / r_a))} \quad (1.2)$$

where R_n is the net radiation flux at the surface, G is the soil heat flux, ρ is the air density, c_p is the specific heat of moist air, $(e_s - e_a)$ is the vapour pressure deficit, r_c is the crop canopy resistance, r_a is the aerodynamic resistance, Δ is the slope vapour pressure curve, γ is the psychrometric constant, and λ is the latent heat of vaporization.

The calculation of net radiation is based on a radiation balance, including a model for the exchange of net thermal radiation:

$$R_n = (1 - \alpha) S_i + f_c (\varepsilon_v (\varepsilon_a - 1)) \sigma T_a^4 \quad (1.3)$$

where α is the surface albedo or canopy reflection coefficient (0.23 overall average for grass), S_i is the global radiation, f_c is an adjustment for cloud cover, ε_a is the effective emissivity of the atmosphere, ε_v is the emissivity of vegetation (0.99 - 0.94) and soil (range 0.98 - 0.80, default value 0.98), σ is the Stefan-Boltzmann constant ($4.90 \cdot 10^{-9} \text{ [MJ m}^{-2} \text{ K}^{-4} \text{ d}^{-1}]$), and T_a is the mean air temperature. The cloudiness factor is estimated as:

$$f_c = a_c \frac{S_i}{a_s S_e} + (1 - a_c) \quad (1.4)$$

where S_e is the extraterrestrial radiation and a_c and a_s are empirical constants ($a_c=1.36$ and $a_s=0.75$, FAO, 1990). The value $a_s=0.75$ indicate that the clear sky radiation corresponds to 75% of the extraterrestrial radiation. The atmospheric emissivity can be estimated from a number of different models, viz. Brunt (1932), Brutsaert (1975), Swinebank (1963), Idso and Jackson (1969), and Satterlund (1979). The default model in Daisy is the Brunt formula:

$$\varepsilon_a = a_e + b_e \sqrt{e_a} \quad (1.5)$$

where the standard parametrization $a_e=0.64$ and $b_e=0.14$ (FAO, 1990) is adopted as default.

The aerodynamic resistance for the reference vegetation is estimated as:

$$r_a = \frac{208}{u_2} \quad (1.6)$$

where u_2 is the wind speed at 2 m. The corresponding canopy resistance is assumed to be $r_c=70$ s/m (FAO, 1990).

The extraterrestrial radiation is estimated as:

$$S_e = G_{sc} d_r (\omega_s \sin \varphi \sin \delta + \cos \varphi \cos \delta \sin \omega_s) / \pi \quad (1.7)$$

where G_{sc} is the solar constant, d_r is the relative Earth - Sun distance, δ is the solar declination, φ is the latitude, and ω_s is sunset hour angle. The relative Earth - Sun distance is:

$$d_r = 1 + 0.033 \cos \left(\frac{2\pi}{365} t \right) \quad (1.8)$$

where t is the Julian day or the number of the day in the year. The sunset hour angle is:

$$\omega_s = \arccos(-\tan \varphi \tan \delta) \quad (1.9)$$

and the solar declination is:

$$\delta = 0.409 \sin \left(\frac{2\pi}{365} t - 1.39 \right) \quad (1.10)$$

It is noted that the implemented version of the FAO reference evapotranspiration requires knowledge of global radiation, air temperature, air humidity and wind speed.

The minimum data set required in order estimate potential evapotranspiration is global radiation and air temperature. In this case the Makkink equation is applied to estimate a reference evapotranspiration for a surface of short grass (Hansen, 1984):

$$E_r = 0.7 \frac{\Delta}{\Delta + \gamma} \frac{S_i}{\lambda} \quad (1.11)$$

The model can make use of either hourly or daily data. If daily data are used, then the potential evapotranspiration is distributed over the day in accordance with the distribution of the extraterrestrial radiation.

Surface Water Balance.

The objective of the surface water balance model is to:

- keep track of water in the canopy interception storage
- calculate evaporation from the canopy interception storage
- calculate through fall
- keep track of surface ponding
- calculate evaporation from the surface ponding storage
- calculate surface runoff
- calculate soil evaporation
- keep track of water stored in snowpack
- calculate evaporation/sublimation from snowpack
- calculate percolation out of snowpack

Input to the surface water balance is precipitation and irrigation. First step is to distribute the precipitation between rain and snow:

$$P_s = \begin{cases} P & T_a \leq T_1 \\ \frac{T_2 - T_a}{T_2 - T_1} P & T_1 < T_a < T_2 \\ 0 & T_2 \leq T_a \end{cases} \quad (1.12)$$

$$P_r = P - P_s$$

where P is the precipitation, P_s is the snow, P_r is the rain, T_a is the air temperature, and T_1, T_2 are empirical constants (default values are $T_1 = -2^\circ\text{C}$ and $T_2 = 2^\circ\text{C}$). If it is snowing or a snowpack is present, then the snowpack model is activated. If this is not the case, then the next step is to activate the interception model. Percolation out of the snowpack or through fall is routed to the ponding model.

It is a basic assumption that “free water”, 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.

Interception

Part of the precipitation and overhead irrigation (e.g. sprinkler irrigation) reaching the top of the crop is intercepted by the crop canopy, which acts as an interception storage. The direct through-fall is assumed to be a function of the leaf area index, and is estimated as:

$$J_{w,d} = P \exp(-K_I L_{ai}) \quad (1.13)$$

where $J_{w,d}$ is the direct through-fall, P is the combined precipitation and overhead irrigation, K_I is an empirical distribution coefficient, and L_{ai} is the leaf area index. Water intercepted by the canopy may be evaporated, stored or flow to the ground as canopy spill off. The evapotranspiration is estimated as:

$$E_I = \text{Min} \left\{ \frac{S_{w,C}^t}{\Delta t} + P - J_{w,d}; E_{p,C} \right\} \quad (1.14)$$

where E_I is the evaporation from the interception storage, $S_{w,C}$ is the storage of intercepted water, $E_{p,C}$ is the potential canopy evapotranspiration and Δt is the time-step. The canopy spill off is estimated as:

$$J_{w,C} = \text{Max} \left\{ \frac{S_{c,C}}{\Delta t} - \left(\frac{S_{w,C}^t}{\Delta t} + P - J_{w,d} - E_I \right); 0 \right\} \quad (1.15)$$

where $J_{w,C}$ is the flow to the ground as canopy spill off, and $S_{c,C}$ is the canopy storage capacity, which is assumed to be proportional to L_{ai} :

$$S_{c,C} = C_i L_{ai} \quad (1.16)$$

where C_i is the interception capacity coefficient (default value $C_i=0.50$ mm, Jensen (1979)) Finally the updated canopy storage is calculated as:

$$S_{w,C}^{t+\Delta t} = S_{w,C}^t + (P - J_{w,d} - J_{w,C} - E_I) \Delta t \quad (1.17)$$

Snow

The model for snow accumulation in the present model is basically adopted from Jansson and Haldin (1980). The basic equations in the model express the conservation of mass:

$$S_{s,S}^{t+\Delta t} = S_{s,S}^t + [P_s + P_r - E_s - J_{w,S}] \Delta t \quad (1.18)$$

$$S_{w,S}^{t+\Delta t} = S_{w,S}^t + [P_r + M - E_s^s - J_{w,S}] \Delta t \quad (1.19)$$

where $S_{s,S}$ is the snow and water in snow storage expressed in equivalent water, $S_{w,S}$ is the water in snow storage, E_s is evaporation plus sublimation from snow storage [mm day^{-1}], E_s^s is the evaporation from snow storage, $J_{w,S}$ is the percolation from snow storage, and M is the snow melting, a negative value indicates freezing.

The evaporation plus sublimation from the snow storage and the evaporation from the snow storage are estimated as follows:

$$E_s = \begin{cases} E_p & E_s \leq P + S_{w,S}^t / \Delta t \\ P + S_{w,S}^t / \Delta t & E_s > P + S_{w,S}^t / \Delta t \end{cases} \quad (1.20)$$

$$E_s^s = \begin{cases} E_s & E_s \leq P_r + S_{s,S}^t / \Delta t \\ P_r + S_{w,S}^t / \Delta t & E_s > P_r + S_{s,S}^t / \Delta t \end{cases} \quad (1.21)$$

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:

$$M^* = (m_t T_a + m_r S_i + q_h / L_m) f \quad (1.22)$$

M^* is the potential snow melting, S_i is the global radiation, q_h is soil heat flux at the surface, L_m is melting heat, m_t and m_r are parameters, and f is constant (1 mm (H₂O) (kg (H₂O) m⁻²)⁻¹)

The influence of temperature on snow melting and freezing in terms of the parameter m_t is expressed by:

$$m_t = \begin{cases} m_t^* & T_a \geq 0 \\ m_t^* \text{Min} \left\{ 1; \left((\Delta Z_s + P / \rho_p) m_f \right)^{-1} \right\} & T_a < 0 \end{cases} \quad (1.23)$$

where m_t^* is a constant (default value $m_t^* = 2.0 \text{ kg m}^{-2} \text{ day}^{-1} \text{ }^\circ\text{C}$), m_f is a constant (default value $m_f = 10 \text{ m}^{-1}$), ΔZ_s is the depth of the old snowpack, and ρ_p is the density of the newly fallen precipitation (snow-rain mixture), which is calculated as a weighted average of the density of water ($\rho_w = 1000 \text{ kg m}^{-3}$) and powder snow ($\rho_s = 100 \text{ kg m}^{-3}$):

$$\rho_p = \rho_w + (\rho_s + \rho_w) \frac{P_s}{P} \quad (1.24)$$

The influence of global radiation on snow melting and freezing in terms of the parameter m_r is expressed as:

$$m_r = m_r^* (1 + m_1 (1 - \exp(-m_2 \Delta t_s))) \quad (1.25)$$

where m_r^* , m_1 , m_2 are constants (default values: $m_r^* = 1.5 \cdot 10^{-7} \text{ kg J}^{-1}$, $m_1 = 2.0$, $m_2 = 0.1 \text{ days}^{-1}$), and Δt_s is the age of surface snow (days since last snow fall).

The actual snow melting and freezing is then estimated as:

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

$$M_1 = - (S_{s,S}^t / \Delta t + P_r - E_s^s) \quad (1.26)$$

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

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

$$S_{c,S} = f_c \left(S_{s,S}^t + (P - E_s) \Delta t \right) \quad (1.27)$$

where $S_{c,S}$ is the storage capacity of snow storage for retention of liquid water, and f_c is the capacity coefficient of snow storage for retention of liquid water. The percolation of water out of the snow storage is estimated as:

$$J_{w,S} = \text{Max} \left\{ 0; S_{w,S}^t + (P_r - E_s + M) \Delta t - S_{c,S} \right\} / \Delta t \quad (1.28)$$

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

$$\rho_{s,p}^{t+\Delta t} = \text{Max} \left\{ \rho_{s,p}^t; \rho_s + \rho_l \frac{S_{w,S}^{t+\Delta t}}{S_c} + \rho_2 S_{s,S}^t \right\} \quad (1.29)$$

where $\rho_{s,p}$ is the density of snowpack, and ρ_1 and ρ_2 are constants (default values $\rho_1 = 200 \text{ kg m}^{-3}$, $\rho_2 = 0.5 \text{ m}^{-1}$).

Ponding.

Through fall, percolation out of the snowpack, and rain or irrigation directly reaching the soil surface may be stored on the surface as ponding. This only occurs if the inputs exceed the surface evaporation plus the infiltration. If ponding occurs, surface runoff may be initiated. This happens if the ponding exceeds a certain threshold characterizing the surface depression storage. The surface runoff is simulated by a simple linear model:

$$q_p = \text{Max} \{0; k_p (S_p - S_d)\} \quad (1.30)$$

where q_p is the surface runoff, k_p is a runoff coefficient, S_p is the ponding, and S_d is the surface depression storage capacity. When ponding occurs, then the infiltration is simulated by soil water model. In all other cases, the infiltration is determined by the rate at which water is allocated to the surface.

Soil Evaporation and Transpiration.

When PET exceeds the evaporation from free water surfaces at the surface soil, evaporation or transpiration may take place. 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):

$$E_{p,s} = E_p e^{-K_c L_{ai}} \quad (1.31)$$

where $E_{p,s}$ is the potential evaporation from soil surface, E_p is the potential evapotranspiration, L_{ai} is the total leaf area index of the canopy, and K_c is an extinction coefficient (default value $K_c = 0.4$). The actual soil evaporation now depends on the rate at which soil water can be transported to the soil surface:

$$E_s = \text{MIN} \{E_{p,s}; q_e\} \quad (1.32)$$

where E_s is the soil evaporation, and q_e is a potential exfiltration rate, which is determined by the soil water model.

The potential transpiration is calculated as:

$$E_{p,t} = (E_p - E_{p,s}) + \beta (E_{p,s} - E_s) \quad (1.33)$$

where $E_{p,t}$ is the potential transpiration, and β is a transfer coefficient allowing for the transfer of energy from a dry soil surface soil to the canopy (default value $\beta = 0.6$). The actual transpiration is determined by the roots' ability to extract water from the rooting zone.

Soil Water Dynamics

Transport of chemicals within the soil is strongly related to soil water flow. Soil water also acts as a reaction medium for several transformation processes in the soil. In particular such processes as microbial transformation of carbon and nitrogen in soil are strongly influenced by soil water content. Furthermore, soil water flow to root surfaces is a process of significance for plant water uptake as well as for plant nutrient transport to the root surfaces.

The objective of the soil water model is to simulate:

- C Vertical water flow in the unsaturated zone
- C Water flow to root surfaces
- C Soil water content within the unsaturated zone
- C Soil water pressure potential within the unsaturated zone

Vertical water flow, soil water content and soil pressure potential in the unsaturated zone

It is a basic assumption that water flow in the unsaturated zone can take place as Darcy flow within the soil matrix or as gravity flow in distinct macropores (macropore flow). Other forms of preferential flow, e.g. finger flow, are not considered. Hence, the model considers two flow regimes, i.e. a matrix regime and a macropore regime. The matrix flow regime is described by Richards equation (Richard 1931):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K \frac{\partial h}{\partial z} \right] + \frac{\partial K}{\partial z} - S \quad (1.34)$$

where θ is the soil water content, h is the soil water pressure potential, K is the hydraulic conductivity of the soil, and S is a volumetric sink term. A solution to Richard's equation requires knowledge of a relation between θ and h , i.e. a soil water characteristic or retention curve, and knowledge of relation between K and h or θ , i.e. the hydraulic conductivity function. Several models for these relations have been proposed in the literature. The following have been implemented in the Daisy code: the van Genuchten retention curve (van Genuchten, 1980) in combination with Burdine (Burdine, 1952) or Mualem (Mualem, 1976) theory for hydraulic conductivity, the Brooks and Corey (Brooks and Corey, 1964) and the Campbell (Campbell, 1974) also in combination Burdine or Mualem theory. In addition, a modified Brooks and Corey model as proposed by Smith (Smith, 1992) is implemented. Furthermore, it is possible to supply Daisy with the soil hydraulic properties in a tabular form, which makes it possible to use any relation. It should also be noted that the architecture of the Daisy code makes it relatively easy to add new hydraulic models to Daisy.

The Richard's equation is solved numerically in the mixed formulation (Celia and Bouloutas, 1990). The upper boundary condition is determined internally by Daisy (as described above). It may be constituted by a pressure condition when ponding occurs or a flux condition in all other circumstances. The lower boundary is selected by the user. The following conditions are implemented: a pressure condition (known position of the groundwater), gravity flow (deep groundwater), and a lysimeter boundary condition. A special case of a pressure condition is implemented, viz. a pipe drain condition (see below).

If the numeric solution to Richard's equation does not converge within the predescribed number of iterations, the model issues a warning and adopts a simplified soil water model (neglects the second order term in Richard's equation).

The soil water flow is calculated by use of the Darcy equation:

$$q = -K \left(\frac{\partial h}{\partial z} + 1 \right) \quad (1.35)$$

where q is the Darcy flow.

Macropore flow may be initiated at the surface or anywhere within the soil profile provided that macropores are present. Macropore flow is only initiated whenever a certain pressure potential is exceeded. In principle this potential should be 0. However, due to numerical uncertainty a small negative potential is often selected. The default negative potential selected by the model corresponds to half the size of the considered numeric layer. During macropore flow the exchange of water between the soil matrix and the macropores is neglected. Water only enters the soil matrix at the end of the macropore. In the model the macropore system is characterized by a depth at which the macropores begin and a distribution of where they end.

If macropores extend to the surface, macropore flow is initiated whenever ponding occurs. The macropore regime exchanges water with the matrix regime through the S term in Richard's equation.

When the soil begins to freeze, ice is formed. It is assumed that the formation of ice takes place in the large pores of the soil resulting in a movement of water from the small to the large pores. This generates a lowering of the pressure potential in the freezing soil, which again often results in a movement of water from beneath to the freezing zone. This, in combination with the fact that water expands when it is freezing, results in a lowering of the air content of the soil.

As long as air still is present in the soil, it is assumed that the pressure potential can be found from the soil content of liquid water and vice versa by use of the soil water retention characteristic.

Potential exfiltration rate

The amount of soil water which can be transported to the soil surface is estimated as:

$$q_e = -\frac{K}{C_\theta} \left[\frac{\partial \theta}{\partial z} \right]_{z=0} \quad (1.36)$$

q_e is the exfiltration rate or Darcy flow velocity towards soil surface, and $C_\theta (=d\theta/dh)$ is the specific water capacity. The gradient $\partial\theta/\partial z$ is estimated on the assumption that $\theta = 0$ at $z = 0$.

Extraction of soil water by roots

The calculation of the extraction of soil water by plant roots is based on the following assumptions: i) the root extracts water from a cylindrical soil volume around it and the radius of this volume corresponds to half the average distance between roots; ii) flow towards the root is radial and can be described by the Darcy equation; iii) the pressure potential at the outer boundary of the considered soil cylinder equals the bulk pressure potential as obtained from the solution to Richard's equation; iv) the potential drop towards the root surface can be approximated by a series of steady state profiles; v) the plant determines the pressure potential at the root surface, however this potential is limited by the permanent wilting point; vi) at the root surface a contact resistance exists, which can be evaluated according to Herkelrath *et al.* (1977). These assumptions lead to the following expression:

$$S_r = 4\pi L \frac{\theta_r}{\theta_s} \frac{M(h) - M(h_r)}{-\ln(r_r^2 \pi L)} \quad (1.37)$$

where S_r is a volumetric sink term (water uptake by roots), L is the root density, θ_r is soil water

content at h_r , θ_s is the soil water content at saturation, h_r is the soil water pressure potential at the root surface, r_r is the root radius, and M is the matrix flux potential, which is a function of the pressure potential:

$$M(h_p) = \int_{-\infty}^{h_p} K dh \quad (1.38)$$

During a simulation L , r_r , h and hence $M(h)$ are known, while S_r , h_r and hence θ_r and $M(h_r)$ are unknown. Two different situations can occur:

- C transpiration at a potential rate
- C transpiration at a lower rate than the potential rate

In the first situation it is the climatic conditions that determine the water uptake by the plants. In this situation it is assumed that an unknown pressure potential exists at the transition between root and shoot (ψ_x). Based on this pressure potential, ψ_x , the pressure potential at the root surfaces is calculated:

$$h_r = \psi_x + R_x z \quad (1.39)$$

where R_x is a transport resistance coefficient. The task is then to find the value of the pressure potential ψ_x by iteration so that the following condition is fulfilled:

$$E_t = \int_0^{z_r} S_r dz \quad (1.40)$$

where $E_t = E_{p,t}$ is the transpiration of the crop and z_r is the rooting depth.

In the second situation it is assumed that it is the transport of water from the bulk soil to the root surface that determines the water uptake. In this case, it is assumed that a common pressure potential exists along the root (h_r) and that the value of h_r can be equated by the pressure potential at wilting point.

Pipe drains.

When pipe drains are present, it is assumed that an aquitard is located beneath the pipe drains and that the deep percolation through the aquitard can be calculated as:

$$q_a = K_a \frac{H_p - H_a}{\Delta z_a} \quad (1.41)$$

where q_a is the percolation through the aquitard, K_a is the hydraulic conductivity of the aquitard, Δz_a is the size of the aquitard, H_a is the pressure potential in the aquifer beneath the aquifer measured at the transition between the aquifer and the aquitard, and H_p is the height of the groundwater table above the aquitard.

When the groundwater table is located above the pipe drains, it is assumed that the drain flow can be estimated by Hooghoudt's equation:

$$q_e = \frac{4K_1 H^2 + 2K_2 H d}{L \Delta x - \Delta x^2} \quad (1.42)$$

where q_e is an equilibrium drain flow, K_1 is the hydraulic conductivity in the saturated soil above

drain depth, K_2 is the hydraulic conductivity in the saturated soil between drain depth and the aquitard, d is the vertical distance between drain depth and the aquitard, L is the horizontal distance between pipe drains, Δx is the horizontal distance from the drain pipe, and H is the horizontal distance between the pipe drains and the groundwater table. K_1 is estimated as a weight-average of the hydraulic conductivities of saturated soil horizons above the drain. The weight factors are based on the thickness of the considered soil layers. K_2 is calculated in a similar way for the soil horizons below the drains. It is noted that this is valid only for steady state conditions. Hence, the pipe drain model is an approximation assuming a series of steady states.

If the percolation from the unsaturated zone, q_z , exceeds the combined flux, $q_a + q_e$, then it is assumed that the groundwater table is rising and a new position of the groundwater table is calculated. Otherwise, the groundwater is falling, and also in this case the position of the groundwater table is adjusted.

The flow to drain pipes within a time step is equated to the equilibrium drain flow. The flow to drains within a soil layer is simulated by a volumetric sink within the layer:

$$S_d = \frac{q_e}{\Delta z} \left[\frac{K \Delta z}{\sum K \Delta z} \right] \quad (1.43)$$

where S_d is the sink term of the considered soil layer, Δz and K are the corresponding layer thickness and hydraulic conductivity, respectively, and $\sum K \Delta z$ is the sum of conductivity times layer thickness for all considered layers.

SOIL HEAT BALANCE

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. Thus the objective of the heat model is to provide soil temperature for abiotic functions governing biological processes described in other submodels of DAISY.

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 soil constituents. In this approach it is a basic assumption that each small unit cell of soil contains a representative sample of soil constituents.

Heat flow equations

Conservation of heat, including phase change due to freezing or melting, yields:

$$\frac{\partial (C_s T)}{\partial t} - L_f \rho_i \frac{\partial x_i}{\partial t} = - \frac{\partial q_h}{\partial z} - S_h \quad (1.44)$$

where C_s is the volumetric heat capacity of soil, T is the soil temperature, L_f is the latent heat of fusion, ρ_i is the density of ice, x_i is the volumetric ice content, q_h is the heat flux density, and S_h is a heat sink (when plant roots extract water, heat is removed from the system too).

One dimensional combined heat transfer due to conduction and convection:

$$q_h = -K_h \frac{\partial T}{\partial z} + c_w \rho_w T q \quad (1.45)$$

where K_h is the thermal conductivity of the soil, c_w and ρ_w are the specific heat capacity and density of water, respectively, and q is the water flux density. Combination of the heat conservation equation and the heat transfer equation, introduction of water conservation, and assuming that $S_h = c_w \rho_w S_r T$ where S_r is the volumetric water uptake by roots leads to the following equation:

$$C_s \frac{\partial T}{\partial t} - [L_f + (c_w - c_i)T] \rho_i \frac{\partial x_i}{\partial t} = K_h \frac{\partial^2 T}{\partial z^2} + \left[\frac{\partial K_h}{\partial z} - c_w \rho_w q \right] \frac{\partial T}{\partial z} \quad (1.46)$$

It is noted that the transport of heat in macropores has been neglected. When freezing or thawing takes place, soil water exists in equilibrium with ice at a temperature below the normal freezing point of bulk water. This was due to the effects of capillary and osmotic forces. In addition, the ice pressure exerted by the expansion of freezing water influences the freezing process. It is assumed that the freezing point depression in the soil can be described as proposed by Miller (1980):

$$T = 273 \frac{\frac{\psi - \pi}{\rho_w} - \frac{P_i}{\rho_i}}{L_f} \quad (1.47)$$

where ψ is the soil water pressure potential ($\psi = gh$, where g is the acceleration of gravity), π is the osmotic potential, and P_i is the ice pressure. During freezing the freezing point depression is often dominated by the effect of the capillary forces, hence all other effects have been neglected. Based on these assumptions and the assumption that $S_r = 0$ when the soil is freezing or melting, the freezing rate can be obtained:

$$\frac{\partial x_i}{\partial t} = \frac{\rho_w}{\rho_i} \left[-\frac{\rho_w L_m C_\theta}{273 g} \frac{\partial T}{\partial t} - \frac{\partial q}{\partial z} \right] \quad (1.48)$$

where $C_\theta (=d\theta/dh)$ is the specific water capacity of the soil. As $L_f \gg (c_w - c_i)T$, it follows:

$$\left[C_s + \alpha \frac{\rho_w^2 L_f^2 C_\theta}{273 g} \right] \frac{\partial T}{\partial t} = K_h \frac{\partial^2 T}{\partial z^2} + \left[\frac{\partial K_h}{\partial z} - c_w \rho_w q \right] \frac{\partial T}{\partial z} - \alpha \rho_i L_f \frac{\partial q}{\partial z} \quad (1.49)$$

where $\alpha = 1$ when freezing or melting takes place or otherwise $\alpha = 0$. It is noted that from a mathematical point of view, the only difference between freezing or melting soil, and the case where no phase change takes place, is a term, which is independent of soil temperature and an apparent very large heat capacity when phase change takes place.

Boundary conditions

Soil surface temperature is assumed to constitute the upper boundary condition. 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 snow is present and the snow contains liquid water, it is assumed that the surface temperature is 0°C. If snow is present and the snow does not contain any liquid water then 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:

$$T_{sf} = \frac{(K_{h1} / z_1) T_1 + (K_s / \Delta z_s) T_a}{K_{h1} / z_1 + K_s / \Delta z_s} \quad (1.50)$$

where T_{sf} is the surface temperature, T_a is the air temperature, T_1 is the soil temperature at z_1 , z_1 is the soil depth, Δz_s is the depth of snow cover, K_{h1} is the thermal conductivity of soil, and K_s is the thermal conductivity of snow, which is estimated according to Corps of Engineers (1956):

$$K_s = \alpha_h \rho_s^2 \quad (1.51)$$

where α_h is an empirical parameter ($\alpha_h = 2.86 \cdot 10^{-6} \text{ W m}^4 \text{ kg}^{-2}$), ρ_s is the density of snowpack.

The lower boundary condition is obtained by an analytical solution to the well-known heat conduction equation:

$$\frac{\partial T}{\partial t} = \frac{K_h}{C_s} \frac{\partial^2 T}{\partial z^2} \quad (1.52)$$

It is noted that this equation is obtained by neglecting transfer of heat by convection and assuming constant C_s and K_h . This equation can be solved analytically with the boundary conditions given by:

$$T(t, 0) = T_{av} + A_t \cos(\omega(t - t_0)) \quad (1.53)$$

$$T(t, \infty) = T_{av} \quad (1.54)$$

where T_{av} is the annual average air temperature at the considered location, A_t is the corresponding amplitude of the annual variation in air temperature, ω is the angular frequency ($2\pi/365 [\text{day}^{-1}]$), t is the day number in the year (Julian day), and t_0 is the day number or Julian day of maximum air temperature ($T(t, 0) = T_{av} + A_t$). Thus the solution is:

$$T(t, z) = T_{av} + A_t e^{-z/d} \cos(\omega(t - t_0) - z/d) \quad (1.55)$$

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

where d is the so-called damping depth and z the depth where the temperature is considered, i.e. the depth of the lower boundary. It is noted that the uncertainty introduced by the lower boundary condition becomes less as the boundary is moved downward in the considered soil profile.

Numerical solution.

The finite difference scheme adopted in the numerical approximation of the heat flow equation is centred in time and space according to the Crank-Nicolson scheme.

Heat capacity of soil

The volumetric heat capacity of a unit cell of soil can be found by addition of the heat capacity of the various constituents of the soil:

$$C_s = x_m \rho_m c_m + x_o \rho_o c_o + x_w \rho_w c_w + x_i \rho_i c_i \quad (1.56)$$

where C_s is the volumetric heat capacity, c is a specific heat capacity, ρ is a density, and x is a fraction by volume. The subscripts m , o , w , and i denotes mineral particles, organic particles, liquid water, and ice, respectively. Most soil minerals have about the same densities and specific heats (de Vries, 1963) therefore the different soil mineral constituents are taken together. It is noted that the contribution from soil air has been neglected due to its insignificant contribution. The specific heat capacity and the density of different soil constituents are given in Table 1.

Thermal conductivity of soil

In Table 1 the thermal conductivity of various soil constituents is given. It appears that large differences in thermal conductivity exist. The 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 flow passes mainly through the grains, but it has to bridge the air filled gaps between the grains around their contact points. When water is present it starts to fill these gaps. 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 bridges are being formed.

Table 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 constituent	ρ kg m ⁻³	c J kg ⁻¹ EC	K W m ⁻¹ EC
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	2.20
Air	1.25	1005	0.025

De Vries (1952, 1963) has developed a physical based model for calculating the thermal conductivity of a soil on the 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. This analogous problem was solved mathematically by Burger (1919). It is a basic assumption that the soil particles can be considered as granules dispersed in a continuous medium.

In moist soils, water can be considered as the continuous medium in which soil particles and air voids are dispersed. 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 the field capacity". Hence water is used 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). In dry soils, air is considered 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 and the wilting point, the thermal conductivity is found by interpolation.

The theory assumes that the shape of soil particles can be described by a so-called formfactor α . For spherical particles: $\alpha=1$; for particles of a shape corresponding to oblate spheroids: $\alpha<1$; for prolate spheroid particles: $\alpha>1$; and finally for flat particles with small thickness, lamellae: $\alpha\rightarrow\infty$. For solid soil particles the spheroid model with a α -value around 4 often can be used (de Vries, 1963).

The theory of de Vries states that the thermal conductivity is calculated from as:

$$K_h = \frac{x_0 K_0 + \sum_{i=1}^N f_i x_i K_i}{x_0 + \sum_{i=1}^N f_i x_i} \quad (1.57)$$

$$f_i = \sum_{j=1}^3 \left[1 + \left(\frac{K_i}{K_0} - 1 \right) g_j(\alpha) \right]^{-1}$$

For spheroids in general $g_2(\alpha)=g_1(\alpha)$ and $g_3(\alpha)=1-2g_1(\alpha)$ are valid. For spherical particles ($\alpha=1$) $g_1(\alpha)=g_2(\alpha)=g_3(\alpha)=1/3$ are valid. For oblate spheroids ($\alpha<1$) $g_1(\alpha)$ is calculated as:

$$g_1(\alpha) = \frac{1}{2} \frac{\alpha^2}{1-\alpha^2} \left[\frac{1}{\alpha^2} + \frac{1}{2\sqrt{1-\alpha^2}} \ln \left(\frac{1-\sqrt{1-\alpha^2}}{1+\sqrt{1-\alpha^2}} \right) \right] \quad (1.58)$$

In the case of prolate spheroids ($\alpha>1$):

$$g_1(\alpha) = \frac{1}{2} \frac{\alpha^2}{\alpha^2-1} \left[-\frac{1}{\alpha^2} + \frac{\pi}{2\sqrt{\alpha^2-1}} - \frac{\arctg(\sqrt{\alpha^2-1})}{\sqrt{\alpha^2-1}} \right] \quad (1.59)$$

In most soils, heat transfer in the air filled pore space does not only take place as thermal conduction, but also by 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 in soil air 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:

$$K_a^* = K_a + K_v \quad (1.60)$$

where K_a^* is the apparent thermal conductivity of soil air, K_a is the thermal conductivity of soil air, and K_v is the thermal conductivity due to vapour transfer. At moisture contents below the wilting point the liquid is held by adsorption forces and the relative humidity is becoming considerably less than 1. Then the transfer of heat by water vapour is restricted. It is assumed that the thermal conductivity due to vapour diffusion can be estimated as:

$$K_v = \begin{cases} K_v^s \theta / \theta_{wp} & \theta < \theta_{wp} \\ K_v^s & \theta \geq \theta_{wp} \end{cases} \quad (1.61)$$

where K_v^s is the thermal conductivity due to vapour diffusion under saturated conditions, θ is the volumetric soil water content ($=x_w$), and θ_{wp} is the volumetric soil water content at $pF = 4.2$. A value of $0.04 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$ for K_v^s was adopted. According to de Vries (1963) this is a reasonable value at a temperature around 10°C .

When the soil is near water saturation soil air forms spherical voids. The influence of the shape factor (g) on the parameter (f) is illustrated in Fig. 2. The minimum influence occurs when $g_1=g_2=g_3=1/3$. As the water content of the soil decreases, air replaces water and subsequently the f -values increase. As it may be seen from Fig. 2 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 which corresponds to $pF = 4.2$. By assuming a linear relation between g_1 and the air content in the region of water content between the saturated condition and $pF = 4.2$ the following equation is obtained:

$$g_1 = 0.333 - (0.333 - 0.070) \frac{\theta_s - \theta}{\theta_s - \theta_{wp}} \quad (1.62)$$

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

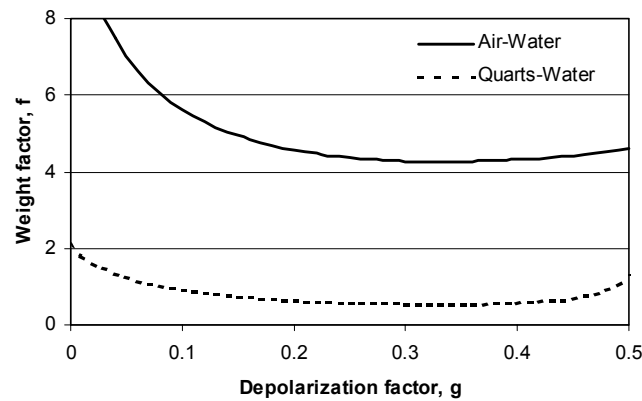


Figure 2. Relationships between the parameter f (weight factor) and the shape factor g_1 for systems with water as the continuous medium and with air and granular of quarts, respectively, as dispersed material.

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 forms small water rings around the contact points of the particles and in a way forms 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.

In frozen soil where the moisture content is below what corresponds to $pF = 4.2$ the same thermal conductivity is used as in the unfrozen situation. At higher water contents the calculations are performed as in the unfrozen case, but the thermal properties of water is now substituted by the thermal properties of ice. In the frozen situation, ice forms the bridges between the solid soil particles instead of liquid water.

De Vries (1952, 1963) has tested the model with good results. He concludes that the accuracy of the estimates is better than 10% in most cases. Kimball et al. (1976) have used de Vries theory in calculating soil heat fluxes in a field of Avondale loam in Arizona. They compared the calculated values with experimental ones. They concluded that "a fair agreement between measured and computed fluxes was obtained only after modifying the air shape factor curve and ignoring heat transfer due to water vapour movement". Kimball et al. (1976) included the variation of K_v^s with temperature. They considered water as the continuous medium over the whole range between oven dry soil and water saturated soil and they used the air shape factor proposed by de Vries (1963). Sepaskhah and Boersma (1979) tested de Vries model for loamy sand, loam, and silty clay loam soils. They found that the model could be used satisfactorily to predict the thermal conductivity of the soil. Hopmans and Dane (1986) also found that de Vries model could be used satisfactorily to predict the thermal conductivity of the soil as the calculated and measured values were within 10%.

For comparing calculated and experimental values of thermal conductivity of soil, we used the de Vries model assuming a porosity of 40%, a quartz fraction of 39%, a fraction of other minerals 19% and an organic fraction of 2%. We further assumed that the form factor of quartz particles corresponded to spheroids with a $\alpha=2.0$, that the form factor of particles of other minerals than quartz corresponded to spheroids with a $\alpha=4.0$ and that the form factor of the organic material corresponded to flat particles with small thickness, lamella. The difference between form factors for quartz and other minerals is based on the fact that quartz often dominates the sand fraction while other minerals dominate the clay fraction of the soil. The field capacity is 0.27 and the wilting point is 0.11. The results are shown in Fig. 3 together with experimental data obtained by Mogensen (1969).

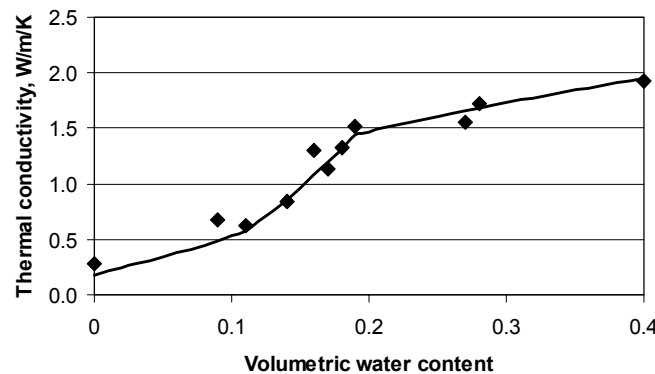


Figure 3. Measured and calculated thermal conductivity of soil related to soil water content.

In Daisy the mineralogical composition of the soil solids is estimated from the textural composition if not otherwise specified. The estimation is based on Møberg *et al.* (1988) and assumes that the quartz content in the sand, silt and clay fraction is 0.70, 0.60, and 0.15 respectively. The adopted default form factors are $\alpha=2.0$ and $\alpha=4.0$ for quartz and other minerals, respectively. The default form factor for organic material is assumed to correspond to lamella.

SOLUTE BALANCE.

The objective of the solute balance model is to keep track of solutes allocated to the system or released within the system. Ammonium, nitrate and pesticide balances are specialisations of the

solute balance. The solute balance comprises a surface balance and a soil solute balance.

Surface solute balance.

Input to the surface solute balance can be in the form of spraying (e.g. pesticides). The amount of water allocated during spraying is typically around 200 L/ha or 0.02 mm, hence the amount of water applied during spraying is considered negligible. During spraying with a certain solute load, a part of the solute may be intercepted by the canopy while another part reaches the soil surface as direct through-fall. The latter is assumed to be a function of the leaf area index and is estimated as:

$$J_{m,d} = P_m \exp(-k_l L_{ai}) \quad (1.63)$$

where $J_{m,d}$ is the through-fall, P_m is the load, k_l is an empirical distribution coefficient (the same as for the surface water balance), and L_{ai} is the leaf area index. A solute intercepted by the canopy may dissipate, be stored, or be washed off. A solute balance on the canopy yields:

$$S_m^{t+\Delta t} = \frac{S_m^t + (P_m - J_{m,d}) \Delta t}{1 + \left(k_l + \frac{f_w J_{w,C}}{S_{w,C}^{t+\Delta t}} \right)} \quad (1.64)$$

where S_m is the amount of stored solute, k_l is a first order dissipation rate coefficient, f_w is a washoff coefficient, $J_{w,C}$ is the flow to the ground as canopy spill off, and $S_{w,C}$ is the storage of intercepted water. The canopy washoff is estimated as:

$$J_{m,C} = J_{w,C} f_w \frac{S_m^{t+\Delta t}}{S_{w,C}^{t+\Delta t}} \quad (1.65)$$

and the dissipation is estimated as:

$$D = k_l S_m^{t+\Delta t} \quad (1.66)$$

where D is the dissipation, which mimics the effects of uptake in the foliar and all loss processes (e.g. photolysis, volatilization).

Soil solute balance

The objective of the soil solute balance is to keep track of how solutes are distributed within the considered soil profile. The model considers sorbed solutes as well as solutes in the soil solution. The model integrates the ongoing transformation processes (losses and gains) and uptake by plants. The core of the solute balance model is the convection-dispersion equation:

$$\frac{\partial (A + \theta C)}{\partial t} = \frac{\partial}{\partial z} \left[\theta D_h \frac{\partial C}{\partial z} - qC \right] + \Phi \quad (1.67)$$

where A is the adsorption, C is the concentration in the soil solution, D_h is the so-called effective dispersion coefficient, θ is the volumetric soil water content, q is the Darcy flow, and Φ is a sink-source term, which integrates transformation processes and plant uptake. The convection-dispersion equation is only valid when so-called local equilibrium is obtained and this condition is not fulfilled when preferential flow takes place. When preferential flow is modeled, then Daisy assumes two flow regimes: a matrix flow regime where the convection-dispersion equation is applied, and a macropore regime where only convection is considered. Exchange between the two regimes is through the sink-source Φ . This exchange is governed by the water flow. The model

does not consider storage of solutes in the macropores, hence the macropores are considered as fast pathway for transport of solutes only.

The adsorption is assumed to be instantaneous (equilibrium approach) and can be described by a Freundlich isotherm or a Langmuir isotherm. The Freundlich isotherm is:

$$A = K_F C^n \quad (1.68)$$

where K_F and n are empirical model parameters. It is noted that if n assumes the value 1 then the Freundlich isotherm becomes linear and the parameter K_F becomes a distribution coefficient. The Langmuir isotherm is:

$$A = \frac{A_{L,m} C}{K_L + C} \quad (1.69)$$

where $A_{L,m}$ is the maximum adsorption capacity and K_L is a half saturation constant.

The effective dispersion coefficient includes the effects of both hydrodynamic dispersion and diffusion, and it is calculated as:

$$D_h = \lambda \left| \frac{q}{\theta} \right| + f_l D_l \quad (1.70)$$

where λ is the dispersivity or dispersion length, D_l is the diffusion coefficient of the solute in free solution, and f_l is a so-called tortuosity factor.

In order to solve the convection-dispersion equation an upper and a lower boundary condition has to be known. The upper boundary condition is always assumed to be a known solute flux through the soil surface and the lower boundary condition is a zero-gradient condition.

The numeric solution to the convection-dispersion equation is based on Wagenet and Hudson (1989).

Vertical movement of a solute in the soil matrix flow regime is a result of convection as well as diffusion:

$$J = -\theta D_h \frac{\partial C}{\partial z} + q C \quad (1.71)$$

where J is the flux density of the solute. If also a macropore-flow regime is active, then transport in the macropores must be added in order to obtain the total solute flux. It is noted that the macropore transport depends on the water flow rate in the macropores and the solute concentration in the region where the macropore flow originated.

Solute movement to root surfaces.

Solutes may be taken up by plants by an active process or by a passive process. If the process is active, it is assumed that the plant regulates the concentration at the root surface of the considered chemical, and that both mass flow and diffusion may contribute to the movement of solutes to the root surfaces. During passive uptake, the movement of solutes to the root surfaces are simulated as pure mass flow.

The transport of solutes from the bulk soil to the root surfaces is based on a number of assumptions similar to those adopted for water flow. Each root may exploit an average effective volume of soil which is assumed to be a cylinder around the root. The radius of this cylinder is assumed to correspond to the average half distance between the roots. If active uptake occurs, it is assumed that solutes are transferred to the root surface by both mass flow and diffusion. Furthermore, it is assumed that the concentration - distance profile around a root develops in time in a stepwise manner, and that at each time-step it approximates to a steady state profile (Baldwin *et al.* 1973). Based on these assumptions the solute-flux towards the root surface is:

$$I = \begin{cases} 4\pi D(C - C_r) \left[\frac{\beta^2 \ln \beta^2}{\beta^2 - 1} - 1 \right] & \alpha = 0 \\ q_r \frac{(\beta^2 - 1)C - \ln(\beta^2)C_r}{(\beta^2 - 1) - \ln(\beta^2)} & \alpha = 2 \\ q_r \frac{(\beta^2 - 1)(1 - \alpha/2)C - (\beta^{2-\alpha} - 1)C_r}{(\beta^2 - 1)(1 - \alpha/2) - (\beta^{2-\alpha} - 1)} & \text{else} \end{cases}$$

$$\alpha = \frac{q_r}{2\pi D} \quad (1.72)$$

$$\beta = (r_r^2 \pi L)^{-1/2}$$

where I is the solute uptake per unit length of the root, D is the diffusion coefficient in the soil, C is the bulk concentration in solution, which is obtained from the solution of the convection-dispersion equation, and C_r is the concentration at root surface, q_r is the water flow towards the root surface, r_r is the root radius, and L is the root density. If the uptake is limited by the availability of the solute then C_r is assumed equal to zero and hence the root acts as a zero sink. In this case total uptake of the solute is calculated by integrating I over the entire root system. In the case of ample solute supply the total solute uptake is determined by the crop demand. In this case total uptake is known and it is distributed over the entire root zone by assuming a common value of C_r to exist along the root surfaces of the entire root system. Soil layers in which $C < C_r$ are assumed not to contribute to the solute uptake. Furthermore, it is assumed that I is limited by a maximum absorption rate, which can not be exceeded.

In the soil, diffusion is influenced by the water content of the soil both in terms of the diffusion cross-section and the tortuous pathway followed by the solute through pores. The bulk soil diffusion coefficient is calculated as:

$$D = \theta D_l f_l \quad (1.73)$$

where θ is the volumetric soil water content, D_l is the diffusion coefficient in free solution, and f_l is a so-called tortuosity factor, which can be estimated in several ways. In Daisy, the following tortuosity factor models have been included: i) step-wise linear model:

$$f_l = \begin{cases} f_l^0 & \theta \leq \theta_0 \\ f_l^0 + a(\theta / \theta_0) & \theta > \theta_0 \end{cases} \quad (1.74)$$

where f_l^0 , θ_0 and a are constants. A value of f_l^0 equal to 10^{-6} is selected arbitrarily, while a and θ_0

are parameters characterizing the soil (default values: $a=2$, θ_0 = soil water content at the permanent wilting point. ii) Millington and Quirk (1960):

$$f_l = \frac{\theta^{7/3}}{\theta_s^2} \quad (1.75)$$

where θ_s is the soil water content at saturation. The Millington and Quirk model is the default model.

NITROGEN BALANCE MODEL

In the soil-plant-atmosphere system nitrogen is present in various forms. The objective of the nitrogen balance model is to keep track of:

- ammonium
- nitrate
- organic matter nitrogen

Exchange between the considered forms and losses from the system may take place due to different processes, viz.:

- immobilization of soil mineral nitrogen by soil microorganisms
- mineralization of organic matter and subsequent formation of ammonium
- nitrification of ammonium and subsequent formation of nitrate
- denitrification of nitrate
- uptake of soil mineral nitrogen and subsequent formation of crop nitrogen
- leaching of ammonium and nitrate

Mineralization-immobilization turnover.

The processes of soil organic matter turnover, mineralization-immobilization turnover or MIT are performed by saprophytic or predatory heterotrophic soil organisms. The soil biomass utilizes nitrogenous organic substances as a source of energy, carbon, nitrogen, etc. If the content of nitrogen in the assimilated organic substance is higher than that required by the biomass for growth, ammonium is excreted to the soil solution. If on the other hand the content of nitrogen in the assimilated organic substance is lower than that required by the biomass for growth, ammonium or nitrate is assimilated from the soil solution and transformed into nitrogenous organic compounds. Hence the net production of ammonium, which is designated net mineralization of nitrogen, is the difference between two opposing processes viz. nitrogen mineralization and nitrogen immobilization.

The activity of the soil biomass and hence the turnover of soil organic matter is usually determined by the availability of the soil organic matter for the soil organisms. The measure used in Daisy for the available organic substrate is the content of carbon in the organic matter. Hence, the simulation of net mineralization of nitrogen is based on the simulation of the turnover rate of soil organic carbon.

The soil organic matter consists of various products which range from intact plant and animal tissues and organisms that live in the soil to black organic material designated humus which is without traces of the anatomical structure of the organisms from which it was derived. Apart from acid soils and poorly drained soils, the C:N ratio in soil organic matter of mineral soil is usually

in the range of 10 to 12.

Soil organic matter and in particular humic substances have long been known to form relatively stable complexes with polyvalent cations, e.g. Al^{3+} , Fe^{3+} , and Ca^{2+} , which by cation bridging can be adsorbed to negatively charged clay surfaces. In this way and by several other mechanisms, the soil organic matter as well as microorganisms may be partly protected against microbial decomposition. For that reason the content of easily decomposable soil organic matter and the soil biomass often increase with increasing clay content of the soil.

In addition to the availability of soil organic matter for the soil biomass, the decomposition rate of organic matter in soil is affected by soil water content, soil temperature, pH, oxygen pressure, and availability of inorganic nutrients. In the pH range of 5 to 8, which is the range typically encountered in agricultural soils, the decomposition rate of organic matter in soil seems unaffected by pH whereas the decomposition rate is limited in acid soils.

In general, the decomposition rate of organic matter in soil is unlimited or only slightly limited by oxygen pressure if the oxygen pressure in the soil air is within the range of 0.05 to 0.2 bar (Parr and Reuszer, 1959; Kempner, 1937). At low oxygen pressure the rate of decomposition of organic matter is low and the decomposition less complete. However, soil aeration and oxygen supply to oxygen demanding processes in the soil, such as root respiration and microbial decomposition, are closely related to soil water content. Hence the aeration conditions may be expressed in term of soil water content. Lack of nitrogen seems to be the only nutrient element, which may limit the decomposition of organic matter in agricultural soils.

In the present soil organic matter model abiotic factors in terms of soil water content, soil temperature, and clay content are taken into account.

Organic matter in soil can be divided into at least three main pools, i.e. dead native soil organic matter (SOM), microbial biomass (SMB), and added organic matter (AOM), Fig. 4. Each of these distinct pools are considered to contain a continuum of substrate qualities, but to facilitate the description of all turnover processes by first-order kinetics each of these main pools has been divided into two subpools: one with a slow turnover (e.g. SOM1, SMB1, and AOM1) and one with a faster turnover (e.g. SOM2, SMB2, and AOM2). First-order kinetics predicts that the decay rate is proportional to the size of the considered pool:

$$\frac{dC}{dt} = -kC \quad (1.76)$$

where C is the carbon content of the considered sub-pool (e.g. SOM1, SMB2, or AOM1) and k is a first-order decomposition rate coefficient, which is modified in accordance with the considered abiotic factors.

The rates of decomposition of SOM1 and SOM2 are considered to be affected by soil temperature, soil water content, and clay content of the soil. In soils with a high input rate of organic matter, SOM2 will increase more rapidly than SOM1 whereas in soils with a low input rate of organic matter, SOM2 will decrease faster than SOM1. Thus the potential nitrogen mineralization rate from dead native organic matter in soil is highly dependent on the distribution of the dead native soil organic matter between SOM1 and SOM2 which in turn is strongly related

to the management history of the soil including in particular previous applications of farmyard manure. The ratio of SOM1:SOM2 is often considered the main calibration parameter of the MIT-model.

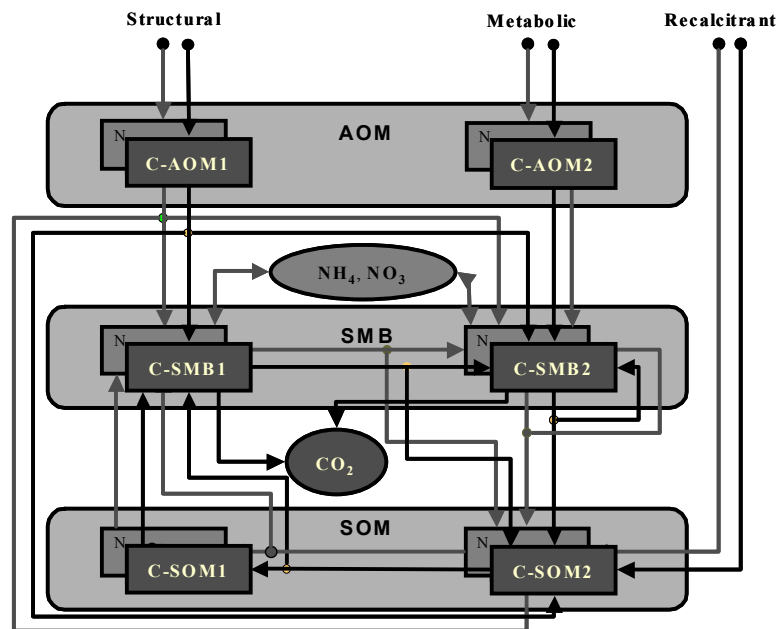


Figure 4. Pools and subpools (1 and 2) of organic matter and related partitioning of organic C (and N) flow between pools. AOM: Added organic matter, SMB: Soil Microbial Biomass, SOM: Soil organic matter.

Production of carbon dioxide results from all C-fluxes into the microbial biomass (SMB) pools (substrate utilization efficiencies being less than unity). Furthermore, microbial maintenance respiration produces carbon dioxide. Maintenance respiration is described by a first order process and is affected by abiotic factors in the same way as the decomposition rates. The decomposition rate of SMB1 is considered to be affected by soil temperature, soil water content, and clay content of the soil, whereas the turnover of SMB2 is considered to be affected only by soil temperature and soil water content. The C:N ratio for SMB1 and SMB2 is assumed to be 6 and 10, respectively, if not otherwise specified. It follows from the interrelationships described, Fig. 4, that the pool size of SMB1 and SMB2 is affected considerably by the size of the substrate pools and especially on the ratio SOM1:SOM2 as the SOM-pools constitute far the most of the organic matter present. However, due to the labile character of the AOM-pools these may have an appreciable impact on the size of the SMB-pools (especially SMB2) just after application of large quantities of organic matter. If not otherwise specified the model will assume that the SMB-pools are in equilibrium with the rest of the system at initialization.

Added organic matter can be organic fertilizers as farmyard manure, slurry, green crop manure, or crop residues left in the field after harvest. In addition, root deposits may be allocated during growth. Furthermore, the model has a routine for bio-incorporation, which moves organic residues from the surface into the soil. Organic matter input to the soil is allocated to two

subpools designated AOM1 and AOM2. The decomposition rates of AOM1 and AOM2 are considered to be affected by soil temperature and soil water content. In case of an organic fertilizer, e.g. farmyard manure, in which some decomposition already has taken place a part of the organic matter is allocated directly to SOM2. The model can work with an undefined number of sets of AOM-pools.

As the flow of matter in the MIT-model is based on C, the corresponding N pools are calculated from the amount of C in the pools using a fixed C-to-N ratio for each pool. Net N-mineralization or N-immobilization is then simply derived from the N-balance. If immobilization occurs, ammonium assimilation has priority over nitrate assimilation. However, neither ammonium nor nitrate can be assimilated by SMB at a rate higher than a specified rate, which is proportional to the concentration of the considered substance. The rate coefficient is a model parameter (default value 0.5 d^{-1})

The abiotic functions used for adjustment of the decomposition rate of soil organic matter at standard conditions to the actual conditions of soil temperature, soil water content, and content of clay, are shown in Fig. 5. It is assumed that no interaction exists between the effect of various abiotic factors and that the combined effect is multiplicative. The abiotic functions were derived from various literature sources, viz. Addiscott (1983), Anderson (1979), Cambell *et al.* (1981), Miller and Johnson (1964), Orchard and Cook (1983), Stanford *et al.* (1973), Stanford and Epstein (1974), Stott *et al.* (1986), Sørensen (1975), and Veen and Paul (1981).

The parameterization of the turnover rates of the SOM-pools and the corresponding partition coefficients (Fig. 4) are obtained by a calibration based on the long term field experiments at Rothamsted Experimental Station, England (Jenkinson and Rayner 1977; Jenkinson *et al.* 1987). The parameterization of the turnover rates of the SOM-pools and the corresponding partition coefficients (Fig. 4) are partly based on incubation experiments (Lind *et al.* (1990)) and partly on field experiments (Muller *et al.* (1997)). MIT-model parameters at standard conditions (optimum water content, 10°C , and no clay content) are shown in Table 2.

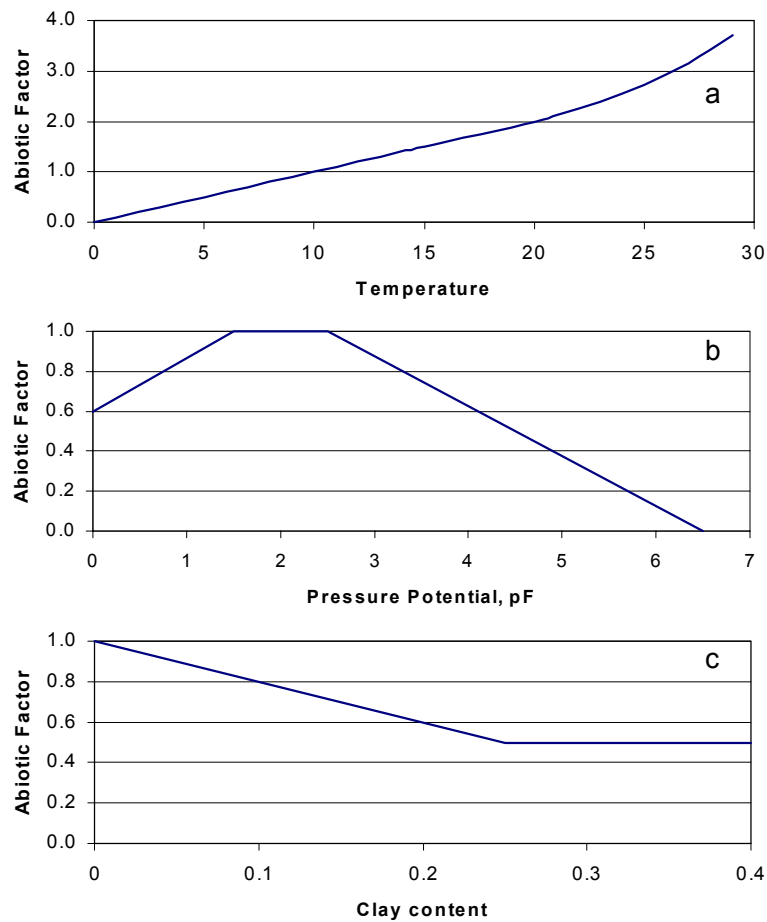


Figure 5. Abiotic functions for adjustment of decomposition rate coefficients to soil temperature (a), content soil water pressure potential (b), and clay (c).

The assessment of the parameters pertaining to long-term simulations has been confirmed by Jensen *et al.* (1997). However, the original parameters pertaining to short-term simulations (Hansen *et al.* 1991a) have been adjusted according to the suggestions Mueller *et al.* (1997) in order to simulate both C and N turnover correctly. The original parameters seem to underestimate the size of the SMB pools.

Parameters for the turnover of AOM-pools depend strongly on the sort of organic material allocated to the AOM-pools. Based on the incubation data of Lind *et al.* (1990), Hansen *et al.* (1990) found the values given in Table 3. It is noted that the assessment of the present parameters is based on incubation experiments in which the added organic material was finely divided, which may have resulted in an overestimation of turnover rates as compared to those expected under usual field conditions. Furthermore, it is noted that the added organic matter contains lignin and other resistant constituents. Thus, it might have been appropriate to route parts of the added organic matter to soil organic matter (SOM2) as in the case of partly humified slurry or manure. Based on field experiments Muller *et al.* (1997) and Muller *et al.* (1998) derived the parameters shown in Table 4.

Table 2. MIT-model parameters adopted from Hansen *et al.* (1990) and Muller *et al.* (1997).

Parameter	Value	Unit
Decomposition rate of SOM1	$2.70 \cdot 10^{-6}$	^a d ⁻¹
Decomposition rate of SOM2	$1.40 \cdot 10^{-4}$	^a d ⁻¹
Decay rate of SMB1	$1.85 \cdot 10^{-4}$	^a d ⁻¹
Decay rate of SMB2	$1.00 \cdot 10^{-2}$	^a d ⁻¹
Decomposition rate of plant material - AOM1 †	$1.20 \cdot 10^{-2}$	d ⁻¹
Decomposition rate of plant material - AOM2 †	$5.00 \cdot 10^{-2}$	d ⁻¹
Maintenance respiration coefficient of SMB1	$1.80 \cdot 10^{-3}$	^a d ⁻¹
Maintenance respiration coefficient of SMB2	$1.00 \cdot 10^{-2}$	^a d ⁻¹
Substrate (SMB) utilization efficiency	0.6	^a
Substrate (SOM1) utilization efficiency	0.4	^a
Substrate (SOM2) utilization efficiency	0.5	^a
Substrate (Plant material – AOM1) utilization efficiency †	0.13	
Substrate (Plant material – AOM2) utilization efficiency †	0.69	
Partitioning coefficient, SOM2 to SOM1	0.1	^a
Partitioning coefficient, SMB1 to SOM2	0.6	^a
Partitioning coefficient, SMB2 to SOM2	0.6	^a
Partitioning coefficient, AOM1 to SMB1 †	0.5	
Partitioning coefficient, AOM1 to SMB2 †	0.5	
C/N ratio of SOM1 (depending on soil-SOM)	8-14	
C/N ratio of SOM2 (depending on soil-SOM)	8-14	
C/N ratio of SMB (SMB1 & SMB2)	6.7	^a
C/N ratio of AOM1 (depending on input material)	1-100	
C/N ratio of AOM2 (depending on input material)	1-100	

† Based on decomposition of rape straw (Muller *et al.* (1997)).

^a The value is included as a default value in the Daisy code

Table 3. Values of parameters for added organic matter to soil in the soil organic matter model assessed from short-term incubation experiments (Hansen *et al.* (1990) based on Lind *et al.* (1990)). Substrate utilization efficiency $E=0.60$. The [C/N] ratio of AOM2 is calculated from the C and N balances of the substrate.

Organic Matter	k_{AOM1}^* day ⁻¹	k_{AOM2}^* day ⁻¹	f_{AOM1}	f_{AOM2}	[C/N] _{AOM1}	$f_{AOM16SMB1}$	$f_{AOM16SMB2}$
Plant residues †	$5.0 \cdot 10^{-3}$	$5.0 \cdot 10^{-2}$	0.40	0.60	80	0.50	0.50
Straw	$1.0 \cdot 10^{-2}$	$1.0 \cdot 10^{-1}$	0.45	0.55	80	0.50	0.50
Pig Slurry	$5.0 \cdot 10^{-3}$	$1.0 \cdot 10^{-1}$	1.00	0.00	80	0.45	0.45

† Grass

Table 4. Specification of C partitioning and C/N ratios of AOM-pools (Muller *et al.* (1997); Muller *et al.* (1998)).

	f_{AOM1}	f_{AOM2}	$[\text{C/N}]_{\text{AOM}}$	$[\text{C/N}]_{\text{AOM1}}$	$[\text{C/N}]_{\text{AOM2}}$
Rape Straw	0.96	0.04	80	92	19
Barley Straw	0.94	0.06	72	110	12
Blue Grass	0.88	0.12	22	25	12
Maize	0.77	0.23	32	37	23

Nitrification

The microbial process whereby ammonium is oxidized into nitrate is referred to as nitrification. In well aerated arable soils, at relatively high water content ($1.5 < \text{pF} < 2.5$), pH in the range of 4-8, soil temperature higher than 5°C, the microbial activity is limited by the availability of organic carbon, and most ammonium is oxidized into nitrate as rapidly as it is formed by the process of ammonification. Thus under such conditions, nitrite is rapidly oxidized into nitrate, and the release of N_2O during oxidation of ammonium in all probability occurs only under conditions of reduced oxygen pressure. Under such conditions, no oxygen stress, nitrification can be considered as a single step process which in Daisy is described by a Michaelis-Menten type kinetics:

$$\xi_n = \frac{V_n(T, h) N_{am}}{K_n + N_{am}} \quad (1.77)$$

where ξ_n is the specific nitrification rate, $V_n(T, \psi)$ is the maximum nitrification rate, N_{am} is the ammonium concentration in soil, K_n is a half saturation constant, T is the soil temperature, and h is the pressure potential of soil water.

Abiotic factors affecting nitrification in soils are substrate (NH_4^+ , O_2 , CO_2) concentrations, pH, temperature, and soil moisture content (Focht and Verstraete, 1977). In addition naturally occurring inhibitory substances may affect the nitrification. There is no evidence that pH in the range of 5.5-8.0 and concentrations of CO_2 are ever limiting the nitrification process whereas the concentration of O_2 clearly can be limiting. As in the MIT-model, the aeration conditions are expressed in terms of the soil water content. The abiotic factors are assumed only to affect the maximum nitrification rate:

$$V_n(T, h) = V_n^* F_n^T(T) F_n^h(h) \quad (1.78)$$

where V_n^* is the maximum nitrification rate at 10°C and optimum soil water conditions, $F_n^T(T)$ is the soil temperature function (Fig. 6), and $F_n^h(h)$ is pressure potential function (Fig. 6). The adopted abiotic factors shown in Fig.6 were derived from the following sources: Flowers and O'Callaghan (1983), Tyler *et al.* (1959), Addiscott (1983), Miller and Johnson (1964), Sabey (1969), and Reichman *et al.* (1966). Comparing Fig. 5 and Fig. 6, it appears that ammonium accumulation may occur at low temperatures and at low and high soil water contents.

Two versions of the nitrification model are implemented in Daisy. In the default version the ammonium concentration is based on the volume of soil (default parameters: $V_n^* = 5 \text{ g m}^{-3} \text{ d}^{-1}$ and $K_n = 50 \text{ g m}^{-3}$). The other version is based on ammonium concentrations in the soil solution.

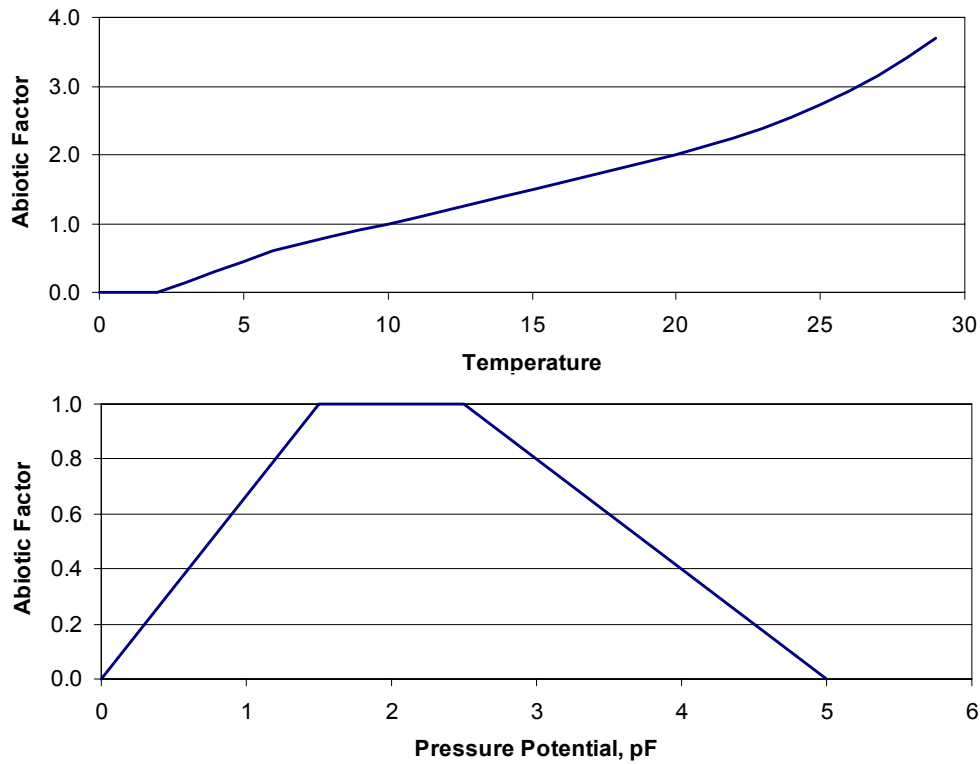


Figure 6. Abiotic functions for adjustment of nitrification rate coefficients to soil temperature (top), and soil water pressure potential (bottom).

Denitrification

Biological denitrification has long been considered an important pathway by which nitrogen is lost in the form of gaseous nitrogen oxides or nitrogen gas from the soil to the atmosphere. Although biological denitrification has been studied extensively during the recent two decades, lack of knowledge still exists about the quantification of biological denitrification under field conditions from fundamental microbial processes. However, it is well established (Fillery, 1983) that the rate of denitrification is related to the amount of easily decomposable organic matter, the volume of anaerobic micro sites within an otherwise aerobic media, the soil temperature, and the concentration of nitrate in the soil solution.

In the present model, denitrification is simulated by means of a rather simple index type model taking into account the decomposition of organic matter, volume of anaerobic microsites expressed simply in terms of soil water content, soil temperature, and the concentration of nitrate in soil solution. In accordance with Lind (1980) the potential denitrification rate (the rate anoxic conditions and ample nitrate concentration) of the soil is expressed as a linear function of the CO_2 evolution rate:

$$\xi_d^* = \alpha_d^* \xi_{\text{CO}_2} \quad (1.79)$$

where ξ_d^* is the potential denitrification rate of soil, ξ_{CO_2} is the CO_2 evolution rate simulated by the MIT-model, and α_d^* is an empirical constant (default value 0.1 g Gas-N/g CO_2 -C). In the present model, the values of ξ_{CO_2} are derived from the organic matter model as the evolution of

CO₂ from the decomposition of organic matter.

The actual denitrification rate is determined either by the transport of nitrate to the anaerobic micro sites or the actual microbial activity at these sites. Transport of nitrate to the denitrifying micro sites is a diffusion process. Hence the maximum transport will take place when the micro sites act as zero sinks. The maximum transport of nitrate to micro sites can therefore be assumed to be proportional to the nitrate concentration in the soil ($N_{ni} = \theta C_{ni}$, where C_{ni} is the concentration in the soil solution). The increased tortuosity when the soil dries is of little consequence as denitrification is very limited in dry soil. In the case of ample supply of nitrate, the actual denitrification rate is determined by multiplying the potential denitrification rate by a modifier function. Hence, the actual denitrification can be simulated as:

$$\xi_d = \text{Min} \{ F_d^\theta(\theta) \xi_d^*; K_d N_{ni} \} \quad (1.80)$$

where ξ_d is the actual denitrification rate, $F_d^\theta(\theta)$ is a modifier function, and K_d is an empirical proportionality factor (default value: d⁻¹). The modifier function is assumed to be a function of the soil water content and is adopted from Rolston et al. (1984), Fig. 7.

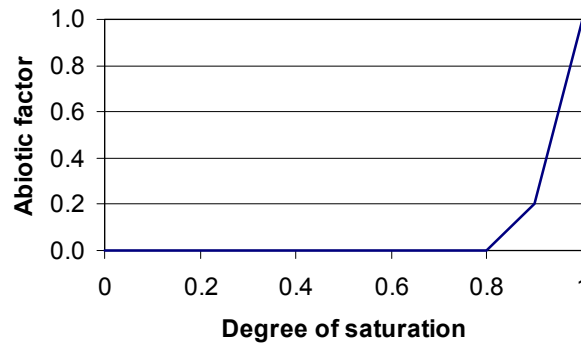


Figure 7. Soil water content modifier function for adjustment of denitrification rate

Nitrogen uptake by plant.

The nitrogen uptake model is based on the concept of potential nitrogen demand, which is simulated by the crop model. The actual nitrogen uptake is either determined by this potential demand or by the availability of nitrogen in the rooting zone, i.e. the rate at which nitrogen can be transported to the root surfaces and subsequently taken up by the root system. The simulation of transport to root surfaces is described in the section on solute transport. The plant may take up nitrogen in the form of either ammonium or nitrate. In the model it is assumed that uptake in the form ammonium has priority over uptake in the form nitrate. However, as ammonium generally is strongly sorbed in most soils most of the uptake normally takes place as nitrate.

Sorption of ammonium may be simulated by one of the sorption models included in the solute transport model. At present it is a Freundlich or a Langmuir isotherm. Or it may be simulated by a sorption model based on van Schouwenburg and Schuffelen (1963), which is the default model. The model assumes that a potassium-ammonium exchange takes place at sites located at clay surfaces. The model considers two types of active sites, viz. edge sites and planer sites. The model is given by:

$$A_{am} = x_c \rho_b \left[\frac{V_p C_{am}}{K_p + C_{am}} + \frac{V_e C_{am}}{K_e + C_{am}} \right] \quad (1.81)$$

where A_{am} is the absorbed ammonium, x_c is the clay content of the soil, ρ_b is bulk density of the soil, V_p is the absorption capacity of planer sites of the clay, K_p is the half saturation constant of the planer sites, V_e is the absorption capacity of edge sites, K_e is the half saturation constant of the edge sites, and C_{am} is the ammonium concentration in the soil solution ($V_p = 6 \cdot 10^{-3} \text{ g (g clay)}^{-1}$, $K_p = 63 \text{ g m}^{-3}$, $V_e = 1.8 \cdot 10^{-3} \text{ g (g clay)}^{-1}$, $K_e = 14 \text{ g m}^{-3}$). It is noted that the default ammonium isotherm can be considered as a double Langmuir isotherm.

Leaching.

The leaching of ammonium and nitrate is simulated by the solute transport model and therefore transport in macropores may be included or excluded. However, since ammonium in most cases is strongly sorbed, a no-transport option can be selected in order to save computer time.

Atmospheric deposition and fertilization.

External inputs to the nitrogen balances are atmospheric deposition and fertilization and in certain cases nitrogen moving into the considered soil volume with capillary rise.

The nitrogen deposition is assumed to takes place as wet deposition in the form of ammonium and nitrate dissolved in the precipitation and as dry deposition in the form of ammonium and nitrate adsorbed to solid particles. In the present model the nitrogen deposited is allocated to a surface storage model. When infiltration occurs the nitrogen in the surface storage is released and enters the soil as dissolved ammonium and nitrate in the infiltrating water.

PESTICIDE BALANCE MODEL

The pesticide balance model is a specialization of the general solute balance model. The objective of the model is to keep track of pesticides at the surface and in the soil. Input to the system is due to:

- spraying.

Losses from the system may take place due to:

- effective dissipation, i.e. the effects of uptake in the foliar and all loss processes (e.g. photolysis, volatilization).
- decomposition in the soil
- uptake by plant roots
- leaching

Spraying is an action in the management module of Daisy. The action takes two parameters, viz. a load of pesticide and a pesticide name. The amount of water applied with the pesticide is neglected. The pesticide name is used as an entry in a database of pesticide properties.

Pesticide properties required in relation to the surface balance model are an empirical foliar wash-off coefficient and a lumped dissipation rate coefficient. The former depends on the formulation of the pesticide, e.g. how sticky it is.

Pesticides being washed off the canopy or parsing through the canopy at spraying is assumed to enter the soil. In the soil, pesticides may be sorbed, decomposed, taken up by plants or leached out of the considered soil profile.

Decomposition of pesticides.

Decomposition of pesticides is described by first order kinetics, i.e.:

$$\xi = -[K^* f_T(T) f_h(h) f_{CO_2}(\xi_{CO_2}) f_C(C) f_\tau(\tau)] C_s \quad (1.82)$$

where ξ is the pesticide decomposition rate, K^* is a decomposition rate coefficient, C_s is the pesticide content in the soil, and f_T , f_h , f_{CO_2} , and f_τ are modifier functions responding to the effect of temperature, T , soil water pressure potential, h , carbon dioxide evolution, ξ_{CO_2} , pesticide solute concentration, C , and lag time, τ , respectively. The carbon dioxide evolution is simulated by the MIT-model, and the corresponding modifier function is supposed to account for the general microbial activity in the soil. The default value for this modifier function is 1, i.e. no effect of the general microbiological activity. The modifier function f_C accounts for the influence of the concentration level on the decomposition. The default value is 1, i.e. no effect of the pesticide concentration level. When a pesticide for the first time is allocated to a soil a lag time is often observed before decomposition begins. The lag time modifier function assumes either the value 0 (no decomposition) or the value 1 (decomposition). The lag time, τ , is calculated by the expression:

$$\tau = \text{Max} \left(\text{Min} \left(\sum_{i=t_0}^t g(C_i) \Delta t, 1 \right); 0 \right) \quad (1.83)$$

where t_0 is the time when the pesticide was allocated and t is the present time. The function g depends on the pesticide concentration in the soil solution and yields this effect of the concentration on the development of the lag time. The lag time is scaled and is always in the range of 0 to 1. The modifier function f_τ is 1 if $\tau=1$ in all other cases it is 0. The function g may assume negative values at low pesticide concentrations, thus indicating a loss in the ability of the soil to decompose the considered pesticide. By default the function g assumes the value $1/\Delta t$, indicating that the function f_τ assume the value 1 by default, i.e. by default no lag period is assumed. By default the functions f_T and f_h assumes the values of the corresponding default functions valid for the MIT-model.

Uptake by roots.

Uptake of pesticide by roots is assumed to take place as a passive process, i.e. the pesticide is carried with the transpiration stream to the root surfaces where it is taken up. However, pesticides may not always enter the root when arriving at the root surface, this is described by introducing a reflection coefficient, hence the pesticide uptake is simulated as:

$$I_p = (1 - \rho) q_r C \quad (1.84)$$

where I_r is the pesticide uptake per unit root length, q_r is the transpiration stream or the water flux towards the root surfaces, and ρ is a reflection coefficient (default value $\rho=1$, i.e. no uptake by plant roots of pesticide).

Adsorption transport and leaching

Adsorption is assumed to be instantaneous and can be described by either a Freundlich or a

Langmuir isotherm as described in the solute balance model. Pesticide movement is described in the section on solute balance.

CROP MODEL

The crop model utilizes the Daisy software ability to have multiple formulations of the same model. Daisy includes the original crop model, which has been described in details by Hansen *et al.* (1990) and Petersen *et al.* (1995). In addition a more detailed crop model is included. This model is described in the following.

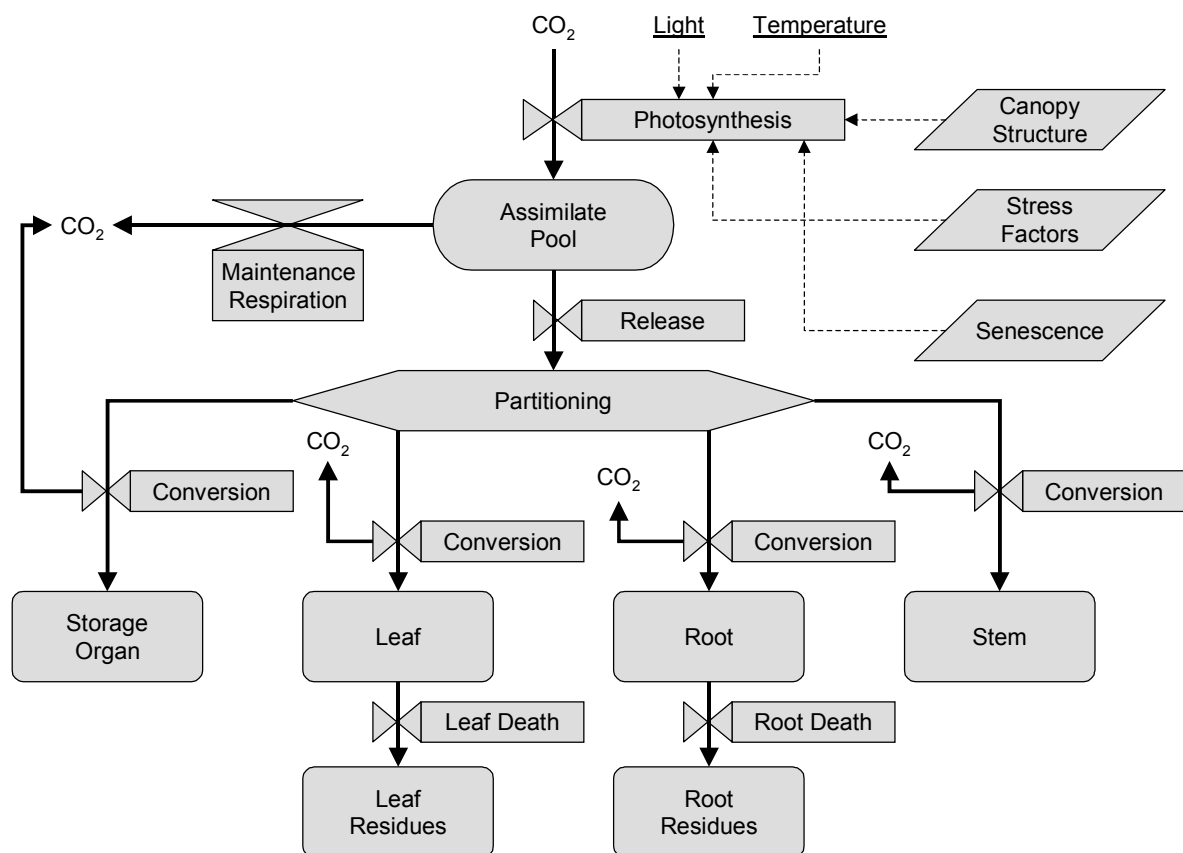


Figure 8. Overview of the carbon flow in the default crop model included in Daisy.

Fig. 8. gives an overview of the carbon flow in the new model. In the figure, solid lines represent flow of matter and the dashed lines represents information flows. Partitioning, leaf and root death, senescence, nitrogen stress (stress factors) a canopy structure are all influenced by the development stage (not shown in the diagram).

Phenological development

The development stage of a crop, DS, quantifies its physiological age and is related to its morphological appearance. In the Daisy crop model DS has the value of 0 at emergence, 1 at flowering and 2 at maturation. The rate of phenological development is influenced by a number of environmental factors. However, the model only takes the effect of temperature and day length into account. The former is assumed to influence the development from emergence (DS=0) to maturation (DS=2), while the latter only may influence the vegetative stage of the crop, i.e. from DS 0 to DS 1. It is a basic assumption that the crop growth per se has no influence on the rate of phenological development.

Daily increments of the development stage, ΔD , are calculated from equation (1.85):

$$\Delta D = d f_t(T_a) f_d(D_l) \quad (1.85)$$

where d is the development rate at reference temperature and reference day length, $f_t(T_a)$ and $f_d(D_l)$ are modifiers accounting for air temperature, T_a , and day length, D_l , respectively. The modifier functions are obtained by linear interpolations between tabulated values of response versus environmental factor. The adopted approach is flexible and allows for a description corresponding to a simple degree-day approach as well as much more complex responses.

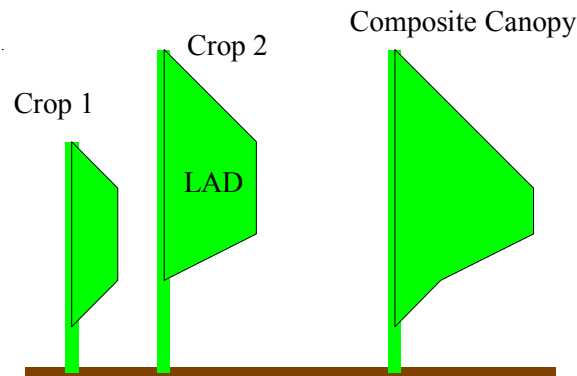


Figure 9. Canopy structure.

Canopy structure

In the model the canopy structure is defined by the leaf area distribution (LAD) as function of plant height, Fig. 9. The leaf area index (LAI) is the integral of LAD over height. LAI is calculated by eq. (1.86):

$$L_{ai} = S_{la} W_{leaf} \quad (1.86)$$

where L_{ai} is LAI, S_{la} is specific leaf area, which is assumed to be a function of DS, and W_{leaf} is leaf weight. Stem and storage organs may also contribute to an efficient LAI. Their contribution is calculated analogous to the contribution from the real leaves using specific area and weight for stem and storage organs, respectively. In addition, a weight factor accounting for the different photosynthetic efficiencies as stem, storage organs and leaf is used in the calculation of the efficient LAI. The weight factor is calculated as the ratio between the photosynthetic rate at saturated light intensity for the stem or storage organ to the corresponding value for the leaf. If necessary parameters are missing, then the contribution from stem or storage organs is neglected. LAD is calculated from efficient LAI and a predefined relative LAD distribution, which is a function of DS. When more than one crop is present the composite canopy LAD is obtained by adding the individual crop LAD distributions, Fig. 9.

Photosynthesis

The photosynthesis model is based on the calculation of light distribution within the canopy (or composite canopy) and single light response curves. The light distribution within the canopy is calculated on basis of Beer's law. The extinction coefficient is assumed to be a characteristic for a given crop and the extinction coefficient for a composite canopy is calculated as a weighted average of the individual crop extinction coefficients. The weight factors are based on the LAI of the individual crops. Reflection coefficients for light are also crop specific and the reflection coefficient for a composite crop is calculated in a similar manner as the extinction coefficient. In the calculation of the light distribution, the canopy is divided into n distinct layers each containing $1/n$ of the total LAI. By applying Beer's law the adsorption of light within layer i , counted from the top of the canopy, can be calculated as:

$$S_{a,i} = (1 - \rho_c) S_{v,0} \left(e^{-k_c(i-1)\Delta L_{ai}} - e^{-k_c i \Delta L_{ai}} \right) \quad (1.87)$$

where $S_{a,i}$ is the absorbed light in layer i , ρ_c is the reflection coefficient of the canopy, $S_{v,0}$ is the incident light above the canopy, k_c is the extinction coefficient and $\Delta L_{ai} = L_{ai}/n$ is the LAI within each canopy layer. When a canopy consists of more than one crop, the absorbed light allocated to each of the crops in a given canopy layer is proportional to the considered crop's contribution to the total LAI within the layer.

Gross photosynthesis is calculated for each individual crop, layer by layer, by applying a light response curve:

$$\Delta F_i = x \Delta L_{ai} F_m \left(1 - \exp \left(- \frac{\varepsilon}{F_m} \frac{S_{a,i}}{\Delta L_{ai}} \right) \right) \quad (1.88)$$

where ΔF_i is the gross photosynthesis for layer i for the considered crop, x is the LAI fraction of the considered crop, F_m is a crop specific photosynthetic rate at saturated light intensity and ε is a corresponding initial light use efficiency at low intensity. F_m is not a constant, but is assumed to be a function of temperature, as illustrated by the indicated influence of temperature on photosynthesis in Fig. 8. The gross photosynthesis is calculated by accumulating the contribution from the individual layers. The time-step in this part of the model is one hour and the produced assimilates are transferred hourly to the carbohydrate reserves, Fig. 8.

Assimilate partitioning, respiration and net production

Respiration is assumed to comprise growth and maintenance respiration (McCree, 1974). Maintenance respiration is assumed to have priority over growth respiration; hence production only takes place if the available carbohydrate reserves exceed the required maintenance respiration. If a surplus of carbohydrate reserves exists, then this surplus is partitioned between the considered crop components, viz. root, stem, leaf and storage organs, and growth respiration is subtracted in order to calculate net production.

Maintenance respiration.

Maintenance respiration is assumed to be proportional to the dry weight of the plant components and each component is assumed to be characterized by a maintenance respiration coefficient, which is temperature dependent:

$$R_m^{component} = r_m^{component}(T) W_{component} \quad (1.89)$$

where R_m is the maintenance respiration, $r_m(T)$ is the maintenance respiration coefficient at the temperature T , and W is the dry weight of the considered crop component. The crop maintenance respiration is the accumulated maintenance respiration originating from the maintenance respiration of the individual crop components.

Assimilate partitioning.

The model only considers determinate crops. Furthermore, it is assumed that stress factors do not influence the assimilate partitioning; hence it can be assumed that partitioning is a function of DS only. In the model the partitioning is described by piecewise linear functions, $\gamma_r(DS)$, $\gamma_s(DS)$, $\gamma_l(DS)$, and $\gamma_o(DS)$, representing the allocation to root, stem, leaf and storage organ, respectively. Note that first $\gamma_r(DS)$ is allocated to the root and then $1-\gamma_r(DS)$ is allocated to the shoot, which is assumed to comprise stem, leaf and storage organs. Then the allocation to the shoot is distributed among stem, leaf and storage organ, hence $\gamma_s(DS)+\gamma_l(DS)+\gamma_o(DS)=1$.

Growth respiration.

The growth respiration rate is assumed to depend only on the end product formed, hence it can be characterized by a conversion efficiency. After subtraction of growth respiration the net production for a specific crop component yields:

$$\left(\frac{\Delta W_{component}}{\Delta t} \right) = E^{component} \gamma^{component} \left(F - \sum_j^{components} R_m^j \right) \quad (1.90)$$

where $(\Delta W/\Delta t)$ is the net production rate, E is the conversion efficiency, γ is fraction of assimilate allocated to the considered crop component ($component = root, leaf, stem, \text{ and } storage \text{ organ}$), F is the assimilate flow from the carbohydrate reserves. F is released from the carbohydrate reserve pool by a linear process.

Senescence

As indicated in Fig. 8, it is assumed that root and leaf material is lost during growth due to senescence and shading. The rate at which matter is lost is assumed to be proportional to the leaf weight. The proportionality factor is divided into two components. One component is assumed to be a piecewise linear functions of DS. Another component, being constant, is only brought into play when the irradiance received by the lower shaded leaves falls below a certain threshold, i.e.

when transmission of light falls below a predefined value, typically around 5 % (Montheith and Unsworth, 1990).

Root production and development

The root system is characterized by root weight, rooting depth, and root density distribution. Root penetration is assumed to take place if the following conditions are fulfilled: 1) daily net root production is positive; 2) the soil temperature at the root tip is above a certain threshold temperature, typically 4°C; and 3) the actual rooting depth is less than a maximum rooting depth. Maximum rooting depth is determined either by the plant species itself or by the chemical or mechanical properties of the particular soil considered. Daily root penetration, $(\Delta d_r/\Delta t)$, is calculated according to Jakobsen (1976):

$$\left(\frac{\Delta d_r}{\Delta t} \right) = \begin{cases} 0 & T_s \leq T_p \\ \alpha_r (T_s - T_p) & T_s > T_p \end{cases} \quad (1.91)$$

where α_r is a root penetration parameter, T_s is the soil temperature at the root tip, and T_p is the threshold temperature. The equation is used for calculation of potential as well as actual root penetration. Potential rooting depth is the rooting depth that would have occurred if the root penetration were not hampered by the soil. The total root length is assumed to be proportional to the root weight. Potential of root density distribution is described in accordance with Gerwitz and Page (1974) assuming that the root density at the potential rooting depth is 0.1 cm cm⁻³. If the actual rooting depth equals the potential one, then the actual root density distribution equals the potential one. If this is not the case, then the actual root density distribution is calculated again by assuming the Gerwitz and Page distribution and setting the root density at the actual rooting depth equal to the density obtained from the potential distribution at this depth.

Water uptake and water stress

The water stress model is based on the assumption that transpiration as well as CO₂ assimilation is governed by stomata responses. Furthermore, it is assumed that stomata is open when intercepted water is evaporated from the leaf surfaces. These assumptions lead to the approximation:

$$F_w = F_p \frac{E_t + E_i}{E_{t,p} + E_{i,p}} \quad (1.92)$$

where F_w is water-limited photosynthesis, F_p is potential photosynthesis, E_t and $E_{t,p}$ is actual and potential transpiration, respectively, and E_i and $E_{i,p}$ is actual and potential evaporation of intercepted water, respectively.

Nitrogen uptake and nitrogen stress

The upper limit for nitrogen uptake by the crop is determined by the difference between a potential nitrogen content, N_c^p , in the crop and the actual nitrogen content in the crop, N_c^a , i.e. $N_c^p - N_c^a$. N_c^p is calculated as:

$$N_c^p = \sum_j^{components} {}^pC_j W_j \quad (1.93)$$

where pC_j is crop specific potential nitrogen concentrations in the considered crop component

($j=\text{root, leaf, stem, and storage organ}$), and W_j is the corresponding dry matter weight. The crop specific potential nitrogen concentrations are functions of DS. The potential uptake determined by the crop demand, U_d , is:

$$U_d = \frac{N_c^p - N_c^a}{\Delta t} \quad (1.94)$$

where Δt is the considered time step. The actual uptake by the crop is calculated as described in the section on Nitrogen Balance. As long as the nitrogen content of the crop, N_c^a , exceeds a certain critical value, N_c^c , no nitrogen stress exists. The critical value is calculated as:

$$N_c^c = \sum_j^{\text{components}} {}^c C_j W_j \quad (1.95)$$

where ${}^c C_j$ is crop specific critical nitrogen concentrations in the considered crop components (root, leaf, stem, and storage organ). The crop specific critical nitrogen concentrations are functions of DS. However, if N_c^a falls below the certain critical value, N_c^c , then nitrogen stress occurs. It is assumed that nitrogen stress influences the gross photosynthesis:

$$F_n = F_w \frac{N_c^a - N_c^n}{N_c^c - N_c^n} \quad (1.96)$$

where F_n is the nitrogen limited gross photosynthesis and N_c^n is a so called non-function nitrogen content of the crop, which are calculated analogous to the critical nitrogen content just replacing the critical concentrations in eq. (1.95) by corresponding non-function concentrations.

MANAGER MODEL

The manager model of Daisy can be considered a special language that allows for building rather complex scenarios of management actions. The management language comprises two different language elements, viz. direct management actions as indicated in Table 5 and conditional statements of the type if-then-else or wait-until etc. The conditional statements make it possible to govern the execution of the management actions, e.g. only allowing irrigation to take place when a certain condition is fulfilled, say when the soil water pressure potential at a given depth is below a certain limit and the crop is within a certain development phase of its life cycle. The construction of the management language also makes it possible to build composite actions based on parameterizations of simple actions. The tillage actions in Table 5 are such composite actions built from parameterizations of the simple actions **swap** and **mix**. The **fertilize** action exists in two versions viz. **fertilize (mineral ...)** and **fertilize (organic ...)**. The key words **mineral** and **organic** cover the description of two very different fertilizer types, viz. mineral and organic fertilizers, respectively. "*Pig Slurry*" is a specialized parameterization of the latter where all the required parameters except the allocated amount of slurry are given in an input library under the heading "*Pig Slurry*". The key words **from** and **to**, taken by the action **fertilize**, indicate that the fertilizer is incorporated in the soil in between the two depths given with the key words.

An example of a simple management scenario is shown in Table 6. The key word **activity** tells the manager that a list of management activities follows. Each activity is executed only once. The left of the table shows the conditional activities and the right of the table shows the direct management activities. From a logical point of view all the activities are at the same level. The

first activity is to wait until the date 1987-03-20 8 a.m. The following activity is to plow. The next activity is again to wait until a certain date and the following activity is to fertilize (100 kg N/ha, where 50% is in the form of ammonium and the rest is in the form of nitrate) and so on. The expression '**crop_ds_after** "*Spring Barley*" 2.0' tells the manager to wait until the spring barley is mature (the development stage 2 is reached) and then to harvest the crop (the next activity). The manager then waits 7 days and incorporates 10 t pig slurry/ha at the depth 10-20 cm.

Building complex management scenarios, including specialized parameterizations of management actions, requires detailed knowledge of the syntax and the key words of the management language. A detailed description is given by Abrahamsen (1999).

Table 5. Important management actions included in the Daisy manager module.

Action	Comment
sow " <i>Spring Barley</i> "	" <i>Spring Barley</i> " is a specialization of the default crop model
harvest " <i>Spring Barley</i> " (stub 5.0) (leaf 1.0) (stem 1.0) (sorg 1.0)	Harvest of spring barley leaving 5 cm stubble and removing all straw (stem), leaf and grain (sorg)
fertilize (mineral (weight 90.0) (NH4-fraction 1.00) (volatilization 0.2))	Applying 90 kg N/ha in ammonium and assuming that 20% is lost as volatilization.
fertilize (" <i>Pig Slurry</i> " (weight 20)) (from -5) (to -15)	Incorporation of 20 t ww/ha of pig slurry (5-15 cm depth). " <i>Pig Slurry</i> " is a specialization of the organic fertilizer model
spray <i>Bentazone</i> 2800	Spraying: 2800 g bentazone/ha
irrigate_surface 30	Surface irrigation: 30 mm
irrigate_top 30	Overhead irrigation: 30 mm
Plowing	Tillage operations are specializations of the primitive actions swap and mix
disk_harrowing	
seed_bed_preparation	

Table 6. A simple management scenario.

(manager activity	
(wait (at 1987 03 20 8))	(plowing)
(wait (at 1987 04 04 8))	(fertilize (mineral (weight 100)) (NH4_fraction 0.50))

```

(wait (at 1987 04 06 8))    (sow "Spring Barley")
                             (sow Grass)

(wait (crop_ds_after
  "Spring Barley" 2.0))    (harvest "Spring Barley")
(wait_days 7)              (fertilize ("Pig Slurry" (weight 10))
                             (from -10) (to -20))

(wait (at 1987 10 01 8))    (harvest Grass (stub 8))
(wait (at 1988 01 04 1))    (stop))

```

CONCLUDING REMARKS

The Soil-Plant-Atmosphere System model Daisy has been described. The objective of the model is to simulate water, heat, and solute balances, and crop production in agro-ecosystems subjected to various management strategies. The included solutes include the nitrogen species ammonium and nitrate and agro-chemicals like pesticides.

The model is especially well suited to model non-point pollution in agricultural watersheds because:

- The model can work in a distributed mode, allowing the simulation of different conditions in terms of soil and agricultural management found within a watershed.
- The model can be linked to a fully distributed hydrological catchment model, allowing the simulation of pollutants in soil, groundwater and surface water.
- The model offers alternative process descriptions for selected processes. The choice of the selected process description is done in the parameterization of the model. The choice can be based on the available information and the available resources in the form of computer time.

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