EXPERT-N

Model Library Documentation

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0 Introduction: Modelling Nitrogen Dynamics in Soil-Plant Systems

0.1 Historical Background

The development of numerical models describing plant growth, water flow and turnover of nutrients in soil-plant systems starts in the late 1960s (Bouman et al., 1996), since then the availabe computer power allowed to simulate plant growth based on processes such as photosynthesis (de Wit, 1965) or solute transport in soils including the processes of convection and diffusion (Frissel et al., 1970; Wierenga and de Wit, 1970; van Genuchten et al., 1974). However, more complex models of the soil-plant system came up only after personal computers had become more and more common at the end of the 1970s and during the 1980s.

After also models to calculate the turnover of soil carbon (C) and nitrogen (N) had been developed in the 1970s (Dutt et al., 1972; Beek and Frissel, 1973; Mehran and Tanji, 1974; Tanji and Gupta, 1978), at the beginning of the 1980s the first models result that combine plant growth with soil water flow, N transport and/or soil C- and N-turnover (Watts and Hanks, 1978; Seligman and van Keulen, 1981). Until mid of the 1980s several models are developed that include approaches still used nowadays as basis for the simulation of agricultural and forest systems such as CENTURY (Parton et al., 1994), NCSOIL (Molina et al., 1983), EPIC (Williams and Renard, 1985), CERES (Jones and Kiniry, 1986; Ritchie et al., 1987), LEACHM (Hutson and Wagenet, 1992), SOILN (Johnsson et al., 1987) and ANIMO (Berghuijs-van Dijk et al., 1985). Whereas these older models were revised, from the end of the 1980s until the mid of the 1990s several new models arise that address the increased request for different applications mainly in the field of agricultural production (Shaffer et al., 2001) with focus on the soil N-transport and N-turnover: HERMES (Kersebaum, 1989), DAISY (Hansen et al., 1990), NLEAP (Shaffer et al., 1991), SUNDIAL (Smith et al., 1996), GLEAMS (Leonard et al., 1987), N-SIM (Engel, 1991a), EXPERT-N (Engel and Priesack, 1993), DNDC (Li et al., 1992), CANDY (Franko et al., 1995), WAVE (Vanclooster et al., 1995).

Based on extensive experimental datasets several model comparisons were accomplished (de Willigen, 1991; Diekkrüger et al., 1995; Tiktak and van Grinsven, 1995). Based on the comparison of simulated with experimental results, in particular comparing time series of crop biomasses and contents of soil water and soil mineral N, general model deficits could be identified, that both concerned all models and only certain models or modelling approaches. However, because of the high model complexity it was in general difficult or even not possible to exactly specify the cause of a certain simulation inaccuracy or modelling error. Often also the resolution in time or space of the experimental data is not high enough to identify model wrongness (Diekkrüger et al., 1995). Therefore, among the models that delivered adequate simulation results were very simple, more empirical models as well as more complex, physically based models (de Willigen, 1991; Diekkrüger et al., 1995). An integrative documentation of 23 N-models (Engel et al., 1993) which served as a basis for the development of EXPERT-N gives a survey on the state of model development for application to agricultural crop systems at begin of the 1990s. A more recent survey can be found in Shaffer et al. (2001), where information on numerous models from Europe, Canada and USA is provided and additionally different model applications are presented, see also Priesack et al. (2001) for an EXPERT-N application therein. In the field of modelling turnover of soil organic substances nine models were evaluated using datasets from seven long-time experiments to compare their prediction capabilities (Smith et al., 1997). A further comparison of models that describe trace gas emissions from soils, in particular N_2O-emissions under agricultural management, showed problems and deficits in establishing an accurate emission prognosis which is needed to determine regional trace gas inventories (Frolking et al., 1998). This model comparison of the four different models CASA-NCASA, DAYCENT, DNDC and EXPERT-N used datasets on soil water and nitrogen contents and N_2O-emissions at four different sites: a dry shortgrass steppe in Colorado USA, a fertilized ryegrass ley cut for silage in Scotland and two cultivated fields in Germany of the FAM Research Network on Agroecosystems (Schröder et al., 2002).

Until the end of the 1980s often simulation and prognosis were focused to determine the change in soil mineral N contents between harvest of the main crop in autumn and sowing of the following main crop in spring, in particular, it was the aim to quantify the amount of nitrate N leached during the winter period in order to correctly size the amount of the first N fertilizer application for the newly growing crop (Engel, 1991b).

During the 1990s N model application was extended to describe the dynamics of soil N pools for the whole vegetation period. This was undertaken mainly to study the impact of different management systems such as different crop rotations or growth of catch crops on soil N dynamics, but also to analyse changes in soil organic matter and to quantify trace gas emissions (CO_2, N_2O, NO) from soils.

Since the end of the 1990s questions about the robustness of model parameterisation are increasingly studied in water flow and solute transport modelling (Schulz et al., 1999), in particular to deal with the observed soil variability (Hupet et al., 2004). Furthermore, N models were extended to describe the impact of preferential flow on nitrate leaching (Larsson and Jarvis, 1999). Facing the change in climatic conditions also questions about the impact of changing precipitation patterns (temporal distribution of occurrence, change of amounts and intensities), changing temperature regimes and changing atmospheric CO_2- and O_3-concentrations are addressed and soil-plant-atmosphere system models are applied for prognosis and scenario studies (Grant et al., 2004).

Moreover, the applied model itself is increasingly object of analysis ranging from the verification of the program code to the intensive testing of the complete model using experimental data. Where as the code verification also has to deal with questions about the correctness and effectiveness of the numerical methods that are applied to solve the model equations, the analysis of the complete model also needs to inspect the way the different model parts are coupled using adequate experimental data sets. Starting with the analysis of single process models and sub-models without considering the mutual dependencies within the complete model, step by step the different couplings and feed-back loops between the different model parts have to be tested. Therefore, highly modular constructed models and model systems such as EXPERT-N are necessary to allow a more thorough model testing and a scientifically based model application, which can also help to assess uncertainties and systematic errors of a process description due to a comparison of different sub-models each representing the same process model as part of the whole model.

0.2 Model Development and Modularity

In the scientific literature the term model is used in different ways. Often under the term model an executable computer program is understood that is based on a mathematical formulation of logical rules and equations and can describe or represent a natural system in a simplified form as part of the reality using input data and parameter values (Refsgaard and Henriksen, 2004). In this sense already the evaluation of a linear regression equation can be seen as a model application that describes a set of experimental data representing a certain part of a natural system. In the following we will understand as a model a finite system of equations and algorithms that represents a dynamical system describing certain aspects of the development of a natural process. However, a dynamical system is not only defined in the strict sense by a system of partial and ordinary differential equations but in a wider sense by a finite series of differential equation systems augmented by a finite set of algorithmic rules. Models that are defined in this way are considered as deterministic or mechanistic models (Addiscott and Wagenet, 1985).

The series of equations and algorithms defining the model can be build up in a way that single components as given by certain sub-series describe a single natural process, e.g. transport of a chemical or growth of a plant organ. This component-wise composition of the model system based on models describing single processes defines the modularity of the model, since the single process models can be considered as elementary modules from which sub-models, e.g. the water flow model or the crop growth model, and finally the total model can be constructed.

This modularity of the model allows a thorough model system analysis starting with the validation of the of the single process model and ending by the comparison of simulation results with experimental data to test the mutual couplings of processes and related feed back loops that determine the total model. Furthermore, model modularity facilitates model extension, since the model can be easily expanded by adding further components and the model can be designed as an open model, which allows the programming user to insert his self-defined and self-programmed sub-models. Such an open and modular model concept was realized by the development of the model system EXPERT-N, resulting in one of the first soil-plant system models with an open and modular model architecture (Abrahamsen and Hansen, 2000). Because of consequently implementing several different sub-models that describe the same single process given by different soil-plant system models such as CERES or LEACHM, from the beginning of the EXPERT-N model development, attention had to be paid to the exchangeability of single process models. Basis of the model development was a documentation and review of known models and modelling approaches (Engel et al., 1993) that lead to the model structure and the partitioning into modular model groups of water flow, heat transfer, solute transport, plant growth and agricultural management and their further division into single process components.

1 Soil Water: Storage and Seepage

1.1 Introduction

The availability of water is one of the prerequisites for the existence of life on earth. Living organisms consist at a major part of water (plants and animals at a fraction of 50-95%) and most physiological processes are closely related to the water phase. At dry land water shortage threatens the living functions of terrestrial organisms within short time, since life cannot exist under dry conditions without regular water uptake to compensate the water losses necessary for cooling. Furthermore, water is needed by terrestrial life not only to build up biomass by assimilation of CO_2, but also to decompose organic substances which happens mainly by micro-organisms in an aqueous environment. Thus, plant canopies consume huge amounts of water (depending on climatic conditions between 10 to 100 m^3 per hectare and day). Communities of living organisms in lakes and rivers, soils and ground water rely on water from which they take up nutrients and energy in form of dissolved organic substances. Therefore, water is also of high importance for the bio-chemical cycling of carbon, nitrogen and other nutrients.

For the hydrological cycle soil is an important water storage. Depending on the soil type one cubic meter of soil contains between 10 to 400 liters of water. Soil type and soil water capacity also determine if the rain water either runs away over the soil surface (run off) and reaches the discharge system as a shock wave possibly contributing to the formation of floods, or if the rain infiltrates into the soil (infiltration) leading to a more steady soil water flow (seepage) and a regular water supply of plants. Additionally, the more steady soil water flow serves as means of transport of solved chemicals including plant nutrients such as ammonium and nitrate. Below the root zone soil water flow usually reaches the groundwater, which in turn feeds the steady water flow of water sources and rivers. The water taken up by the soil partly can return to the atmosphere by evaporation from the top soil or by root water uptake and subsequent transpiration in form of water vapor through the stomata of plant surfaces. Under dry conditions in particular during the summer when precipitation is low and the water uptake by the plant canopy almost exhausts soil water, then the soil hydraulic gradient can cause water flow from wetter soil horizons below the root zone or from groundwater towards the upper dry soil (capillary rise).

Moreover, not only the soil but also the vegetation controls the rate and amount of run off from the soil surface. Water storage at the plant surfaces during and after the precipitation event (interception) reduces the amount of water that hits the soil surface resulting in lower run off and lower infiltration. Comparing different land use systems such as forest, grassland and field, the forest system has an additional water storage due to its mulch layer and the mineral soil generally shows a higher number of macropores that enhance infiltration.

Grassland has no mulch layer and less macropores in the soil. Therefore, the infiltration capacity of grassland soils is lower than that of most forest soils, but it is generally higher than that of crop field soils in which during strong precipitation events a short time soil surface sealing occurs caused by swelling of fine soil particles in the top soil. In this case barely any precipitation water infiltrates and a high run off occurs.

The aim of soil hydrological modelling is to describe the mentioned processes of water flow in the soil-plant-atmosphere system by mathematical means, in a way that it is possible to calculate the dynamics of water exchange between atmosphere, soil and groundwater using as input the data of

- climate and weather conditions as measured by a usual meteorological station,
- basic soil properties including soil bulk density and soil texture and
- land use management e.g. as provided by the farming records

To calculate the water fluxes between atmosphere and the soil-plant system, we estimate the possible water uptake by the atmosphere using the meteorological data and applying a model of potential evapotranspiration. In the model system EXPERT-N different evapotranspiration models are available that are often used for meteorological purposes (DVWK, 1996; VDI, 1993; Smith et al., 1992) such as the models of Penman (VDI), Penman-Monteith (FAO) and Haude (VDI). These approaches can be used depending on available meteorological input data. By coupling with the models of soil water flow and crop growth we can calculate the actual evaporation and actual transpiration from the estimated potential evapotranspiration.

To simulate one-dimensional vertical soil water flow mainly two different approaches are followed (Gilding, 1992; Engel et al., 1993), and either a capacity model or a model based on Darcy-Buckingham's law using a numerical solution of Richards equation is applied. For both approaches additional soil hydraulic parameters are needed. For the capacity model we need data on volumetric water contents at saturation, at field capacity and at the permanent wilting point of each soil horizon. They can be estimated by a discrete pedotransfer function, e.g. according to Renger (1971), from basic soil parameters including bulk density, texture and organic carbon content. For the water flow calculation by Richards equation we need the soil hydraulic functions, i.e. the retention curve and the unsaturated conductivity curve. These curves can be given by parametrisations e.g. according to van Genuchten (1980) and Mualem (1976). If no measured values are available, also in this case pedotransfer functions might be applied to estimate the parameters by using basic soil properties and pedotransfer functions, e.g. according to Campbell (1985), Rawls and Brakensiek (1985) or Vereecken et al. (1989, 1990).

Since under field conditions often preferential water flow in macropores is observed, we additionally included the approach of Durner (1994) in EXPERT-N to simulate water flow in macropores. This preferential flow occurs only in a small fraction of the whole pore volume and is fast compared to the water flow in the remaining pores.
Furthermore, three models to consider water flow during soil freezing conditions (Jansson and Halldin, 1980; Flerchinger and Saxton, 1989; Hansen et al., 1990) have been included into EXPERT-N to obtain an adequate description of soil freezing and thawing. This was achieved by an appropriate model parametrisation and by comparing simulations of the different models with observed data. The models were applied in combination with the N_2O-model to improve simulations N_2O-emissions during freezing and thawing cycles.

1.2 Soil Water Balance

The daily field soil water balance, which describes the daily change of water content ΔW_P $[mm\ d^{-1}]$ stored in a field soil profile P results from

a) the amount of water $Q_{top,P}$ $[mm\ d^{-1}]$, exchanged per day at the soil surface between the soil profile and the atmosphere,

b) the amount of water $Q_{bot,P}$ $[mm\ d^{-1}]$, flowing per day across the lower end of the soil profile, e.g. which leaves or enters the soil profile from the saturated zone,

c) the amount of water S_P $[mm\ d^{-1}]$, extracted per day from the soil profile due to a sink, e.g. by root water uptake:

$$\Delta W_P = Q_{top,P} - Q_{bot,P} - S_P \tag{1}$$

ΔW_P	daily change of water storage in the soil profile P [mm d^{-1}]
$Q_{top,P}$	daily amount of water exchanged across the upper end of the profile P [mm d^{-1}]
$Q_{bot,P}$	daily amount of water exchanged across the lower end of the profile P [mm d^{-1}]
S_P	daily amount of water extracted from the profile P due to a sink [mm d^{-1}]

The amount of water entering or leaving the soil profile can be balanced by quantifying the particular processes determining the water movement from precipitation to groundwater recharge. The water flow rate $Q_{top,P}$ $[mm\ d^{-1}]$ across the soil surface results from the daily precipitation rate PR $[mm\ d^{-1}]$ and irrigation rate IR $[mm\ d^{-1}]$ diminished by: the change rate of interception water IC $[mm\ d^{-1}]$ resting on the vegetation surface; the rate of runoff along the soil surface RO $[mm\ d^{-1}]$; and the actual soil evaporation rate EV $[mm\ d^{-1}]$:

$$Q_{top,P} = (PR + IR - IC - RO - EV) \tag{2}$$

The water flow rate across the lower end of the soil profile is determined by the drainage rate $DR\ [mm\ d^{-1}]$ and by the rate of capillary rise $CR\ [mm\ d^{-1}]$ from the deeper subsurface region, e.g. from the saturated zone:

$$Q_{bot,P} = (DR - CR) \tag{3}$$

The water sink in the soil profile is given by the root water uptake of the plants corresponding to the actual transpiration rate $TR\ [mm\ d^{-1}]$:

$$S_P = TR \tag{4}$$

Adding together the water flow across the upper and the lower boundary of the soil profile and considering the water sink, the following soil water balance results:

$$\Delta W_P = (PR + IR - IC - RO - EV) - (DR - CR) - TR \tag{5}$$

ΔW_P	daily change of soil water storage within the soil profile P $[mm\ d^{-1}]$		
PR	precipitation $[mm\ d^{-1}]$	IR	irrigation $[mm\ d^{-1}]$
IC	interception $[mm\ d^{-1}]$	RO	runoff [mm d^{-1}]
EV	actual evaporation $[mm\ d^{-1}]$	DR	drainage $[mm\ d^{-1}]$
CR	capillary rise $[mm\ d^{-1}]$	TR	actual transpiration $[mm\ d^{-1}]$

1.3 Potential Evapotranspiration

1.3.1 Potential Evapotranspiration from Pan Evaporation Data

1.3.1.1 Daily Potential Evapotranspiration The calculation of the potential evaporation follows the method of Childs and Hanks (1975). It is based on the weekly pan evaporation ET_{pan}^{week} $[mm\ week^{-1}]$ data, that quantify the total evaporation from an open water surface during a week. By applying the crop pan factor k_c [1] of the considered crop species, the daily evapotranspiration ET_{pot}^{day} $[mm\ d^{-1}]$ can be obtained:

$$ET_{pot}^{day} = k_c\ \frac{ET_{pan}^{week}}{7\ d} \tag{6}$$

The empirical crop pan factor k_c [1] relates the pan evaporation to the evapotranspiration of a plant lysimeter, and can be obtained by placing the plant lysimeter next to the evaporation pan. The pan evaporation rate is then compared with the evapotranspiration rate, calculated from the water balance of the lysimeter. As example, the crop pan factor for a grass canopy during winter is given by k_c=0.5 (Haude, 1954).

1.3.1.2 Evaporation and Transpiration The potential daily soil evaporation EV_{pot}^{day} $[mm\ d^{-1}]$ is calculated from the daily evapotranspiration ET_{pot}^{day} $[mm\ d^{-1}]$ and a crop specific soil cover fraction f_{plcv} [1], in order to determine the fraction of the soil surface that is free of plants and plant residues:

$$EV_{pot}^{day} = (1 - f_{plcv})\ ET_{pot}^{day} \tag{7}$$

The potential daily transpiration TR_{pot}^{day} $[mm\ d^{-1}]$ is obtained from the difference between potential daily evapotranspiration ET_{pot}^{day} $[mm\ d^{-1}]$ and the sum of daily actual evaporation from soil EV_{act}^{day} $[mm\ d^{-1}]$ and from interception water EI_{act}^{day} $[mm\ d^{-1}]$ stored on plant surfaces:

$$TR_{pot}^{day} = ET_{pot}^{day} - EV_{act}^{day} - EI_{act}^{day} = f_{plcv} ET_{pot}^{day} + (EV_{pot}^{day} - EV_{act}^{day}) - EI_{act}^{day} \tag{8}$$

1.3.1.3 Distribution During a Day The amount of potential evapotranspiration during the day $ET_p^{[0;1]} = 1.0d\ ET_{pot}^{day}$ is distributed over 12 hours starting at 0.3 day (07h12) and ending at 0.8 day (19h12), where t denotes the time since the start of a new day (0h00), in fractions of the day:

$$ET_p(t) = \begin{cases} ET_{pot}^{day} \pi\ \sin[2\pi(t - 0.3)] & \text{if } 0.3\ \leq t \leq 0.8 \\ 0 & \text{else} \end{cases} \tag{9}$$

The amount of potential evapotranspiration $ET_p^{\Delta t}$ $[mm]$ during the time interval $\Delta t = [t_1; t_2] \subset [0.0;\ 1.0]$ is then calculated by the integral

$$ET_p^{\Delta t} = \int_{t_1}^{t_2} ET_p(\tau) d\tau = f_{\Delta t}\, ET_{pot}^{day} \tag{10}$$

defining the distribution factor $f_{\Delta t}$ $[d]$ for the time interval Δt with τ=0.3:

$$f_{\Delta t} = \begin{cases} \frac{1}{2}\{\cos[2\pi \max(0; t_1 - \tau)] - \cos[2\pi \min(\frac{1}{2}; t_2 - \tau)]\} & \text{for } \Delta t \cap [\tau; \tau + \frac{1}{2}] \neq \emptyset \\ 0.0 & \text{else} \end{cases} \tag{11}$$

Similarly, the potential evaporation $EV_p^{\Delta t}$ $[mm]$ and the potential transpiration $TR_p^{\Delta t}$ $[mm]$ for the time interval Δt are calculated from the daily potential evaporation EV_{pot}^{day}, and daily potential transpiration TR_{pot}^{day}, respectively:

$$EV_p^{\Delta t} = f_{\Delta t}\, EV_{pot}^{day} \quad , \quad TR_p^{\Delta t} = f_{\Delta t}\, TR_{pot}^{day} \tag{12}$$

1.3.2 Potential Evapotranspiration - Penman (VDI) Method

1.3.2.1 Penman Equation If the potential evaporation (e.g. from pan evaporation) cannot be calculated due to the absence of raw data, it can be estimated using the Penman equation (Penman, 1948). This estimation is based on calculations of the energy balance (for radiation energy and vaporation heat) and on aerodynamic considerations (concerning the dependence of evaporation from wind velocity). Climatic input data, such as average daily air temperature T [°C], mean daily relative humidity U $[\%]$, wind speed v $[ms^{-1}]$, cumulative daily solar radiation R_{sol} $[MJ\ m^{-2}\ d^{-1}]$ are required to estimate the daily potential evapotranspiration ET_{pot}^{day} $[mm\ d^{-1}]$ for a grassy surface on a wet soil, or for an open water surface.

The *Penman equation* (DVWK, 1996; VDI, 1993) is defined by:

$$ET_{pot}^{day} = \frac{\Delta}{\Delta + \gamma} \,(\, Rn_s - Rn_l \,)/L + \frac{\gamma}{\Delta + \gamma}\, f(v)\, (\, e_s(T) - e_d \,) \tag{13}$$

ET_{pot}^{day}	daily potential evapotranspiration $[mm\ d^{-1}]$
Δ	slope of the vapor pressure curve $[hPa\ K^{-1}]$
γ	psychrometric constant $\gamma =$ 0.663 $[hPa\ K^{-1}]$
Rn_s	net shortwave radiation $[MJ\ m^{-2}\ d^{-1}]$
Rn_l	net longwave radiation $[MJ\ m^{-2}\ d^{-1}]$
L	latent heat of vaporation $[MJ\ m^{-2}\ mm^{-1}]$
$f(v)$	wind speed function of Dalton $f(v) = 0.27\ (1.0\ +\ 0.864\ v)$ $[mm\ d^{-1}\ hPa^{-1}]$ for the wind speed v $[m\ s^{-1}]$ in 2 m height
$e_s(T)$	saturation vapor pressure $[hPa]$ depending on average daily air temperature T [°C]
e_d	average daily vapor pressure $[hPa]$.

1.3.2.2 Vapor Pressures The saturation vapor pressure $e_s(T)$ $[hPa]$ depends upon the average daily air temperature T [°C](Sonntag, 1994):

$$e_s(T) \;=\; 6.11 \;\; \exp(\, \frac{17.62 \, T}{243.12 \; + \; T} \,) \tag{14}$$

From this expression; the slope of the vapor pressure curve Δ $[hPa \; K^{-1}]$ can be obtained:

$$\Delta \;=\; [e_s(T + 1.0) \; - \; e_s(T)]/(T + 1.0 \; - \; T) \tag{15}$$

The average daily vapor pressure e_d $[hPa]$ is determined from the mean daily relative humidity U $[\%]$ and from the saturation vapor pressure $e_s(T)$ $[hPa]$ by:

$$e_d \;=\; (\frac{U}{100}) \;\; e_s(T) \tag{16}$$

1.3.2.3 Net Radiation Taking into account the albedo α_g [1], which gives the fraction of the short wave radiation reflected by the soil and crop canopy surface, the net short wave radiation is obtained:

$$Rn_s = (\; 1 - \alpha_g \;) \; R_g \tag{17}$$

Rn_s	net short wave radiation $[MJ \; m^{-2} \; d^{-1}]$
α	reflection coefficient or albedo
	overall average for water $\alpha_g = 0.05$ and for vegetation $\alpha = 0.25$ (VDI, 1993)
R_g	global solar radiation $[MJ \; m^{-2} \; d^{-1}]$

The net longwave radiation Rn_l $[MJ \; m^{-2} \; d^{-1}]$ is the effective reflection from the land surface. It results from the difference between thermal radiation from soil and vegetation and the reflected radiation from atmosphere and clouds. It is estimated by the equation of Brunt (1932), see also (Penman, 1948):

$$Rn_l = \epsilon \, \sigma \, (T + 273.15)^4 \; (0.34 \; - \; 0.044 \, \sqrt{e_d} \,) \; (0.1 \; + \; 0.9 \, n/N) \tag{18}$$

Rn_l	net long wave radiation $[MJ \; m^{-2} \; d^{-1}]$
ϵ	emissivity = 0.97 for water surfaces, = 1.0 for other surfaces
σ	Stefan-Boltzmann constant = 4.9 10^{-9} $[MJ \; m^{-2} \; K^{-4}]$
T	average daily air temperature [°C]
e_d	average daily vapor pressure $[hPa]$
n/N	daily relative sunshine fraction $[1]$

1.3.2.4 Latent Heat of Vaporation To transform radiation energy into its equivalent water evaporation, the latent heat of vaporation L $[MJ\ m^{-2}\ mm^{-1}]$ is used and is defined as the energy needed to evaporate 1.0 $kg\ m^{-2}$ water per day, i.e. the energy for the evaporation of 1.0 $mm\ d^{-1}$. L is determined depending on the average daily air temperature T [°C], see DVWK (1996):

$$L \;=\; 2.5 \;-\; 2.42\ 10^{-3}\ T \qquad (19)$$

1.3.2.5 Sunshine Duration The daily sunshine duration n $[h]$ can be estimated from the measured daily solar radiation R_g $[MJ\ m^{-2}\ d^{-1}]$ as follows:

$$n/N \;=\; (R_g/R_a \;-\; A)/B \qquad (20)$$

n	sunshine duration $[h]$
N	maximal possible sunshine duration of the day $[h]$
R_g	cumulative daily solar radiation $[MJ\ m^{-2}\ d^{-1}]$
R_a	cumulative daily extraterrestrial radiation $[MJ\ m^{-2}\ d^{-1}]$
A, B	empirical constants depending on month and site $[1]$

The cumulative daily extraterrestrial radiation R_a $[MJ\ m^{-2}\ d^{-1}]$ and the maximal possible sunshine duration of the day N $[h]$ can be calculated from the latitude ϕ $[Grade]$ $(0°\ ...\ 90°)$ and the number of the day in the year J $[1]$ (1...365), using the solar declination δ $[Grade]$ and the sunset hour angle ω_s $[Grade]$ (VDI, 1993):

$$\begin{aligned} R_a &= 37,5985\ (0,01745\ \omega_s\ sin\phi\ sin\delta \;+\; cos\phi\ cos\delta\ sin\omega_s) && (21)\\ \omega_s &= arccos(-tan\phi\ tan\delta) && (22)\\ \delta &= arcsin(0,3978\ sin(\xi - 77,369 + 1,916\ sin\xi)) && (23)\\ \xi &= 0,9856\ J \;-\; 2,796 && (24)\\ N &= 7,6394\ (0,01745\ \omega_s) && (25) \end{aligned}$$

If for a given location in Germany, the monthly values for the empirical constants A and B are unavailable the values $A = 0,35$ and $B = 0,55$ can be then used for an approximation of R_a and N (DVWK, 1996). Otherwise, the use of daily sunshine duration data n $[h]$ is recommended.

1.3.2.6 Consideration of Different Crop Canopies Empirical crop coefficients k_c $[1]$ are used to calculate the potential evapotranspiration for different agricultural crops or for forest stands. This is achieved by obtaining the product of the reference potential evapotranspiration determined by the Penman formula and the crop coefficient for the crop species being considered:

$$ET_{pot,c}^{day} \;=\; k_c \; ET_{pot}^{day} \tag{26}$$

$ET_{pot,c}^{day}$	daily potential evapotranspiration $[mm \; d^{-1}]$ for the crop canopy
ET_{pot}^{day}	daily potential evapotranspiration $[mm \; d^{-1}]$ acc. Penman
k_c	crop coefficient [1]

The crop coefficient accounts for the canopy height and the soil cover of the crop. For instance, if the canopy does not cover the soil completely, the crop coefficient k_c may be lesser than 1.0. If the crop evapotranspiration is similar to that of low grass, k_c is equal to 1.0. For a fully developed crop, k_c can increase up to 1.5 (DVWK, 1996):

Table 1: Crop Coefficients k_c $[1]$ acc. DVWK (1996)

	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov/Feb
PA	1.00	1.00	1.05	1.10	1.10	1.05	1.05	1.00	1.00
WW	0.90	0.95	1.15	1.35	1.30	1.00	-.-	-.-	0.65
WB	0.95	1.00	1.30	1.40	1.35	-.-	-.-	-.-	0.65
SB	-.-	0.75	1.30	1.40	1.30	-.-	-.-	-.-	-.-
RY	0.85	0.90	1.20	1.30	1.25	0.95	-.-	-.-	0.65
OA	-.-	0.70	1.10	1.40	1.35	0.95	-.-	-.-	-.-
SB	-.-	0.50	0.75	1.10	1.30	1.25	1.10	0.85	-.-
PO	-.-	0.50	0.90	1.10	1.40	1.20	0.90	-.-	-.-

PA	pasture	WW	winter wheat	WB	winter barley	SB	summer barley
RY	rye	OA	oats	SB	sugar beet	PO	potato

1.3.3 Potential Evapotranspiration - Penman-Monteith (FAO) Method

1.3.3.1 Penman-Monteith Equation Based on the Penman equation for estimating the potential evapotranspiration, Monteith (1965, 1981) developed a more complex model, which is now widely used for investigations of soil water flow. To better account for plant canopies, Monteith introduced two additional crop resistance factors: the aerodynamic resistance r_a $[s\ m^{-1}]$ dependent upon wind speed, height and structure of the canopy, and the crop canopy resistance r_c $[s\ m^{-1}]$ related to the stomatal resistance of the plant leaves and reflecting the water supply of the canopy.

The *Penman-Monteith equation* is thus defined:

$$ET_{pot}^{day} = \frac{1}{L^*} \frac{\Delta\,(Rn\,-\,G)\,+\,\rho_a\,c_a\,(e_s\,-\,e_d)/r_a}{\Delta\,+\,\gamma\,(1\,+\,r_c/r_a)} \tag{27}$$

ET_{pot}^{day}	daily potential evapotranspiration $g\ m^{-2}\ s^{-1}]$
L^*	latent heat of vaporation $[MJ\ kg^{-1}]$ (L^*= 2.45 $MJ\ kg^{-1}$ for an average air temperature of 20 °C)
Δ	slope of the vapor pressure curve $[hPa\ K^{-1}]$
Rn	net radiation at the soil surface $[kJ\ m^{-2}\ s^{-1}]$
G	soil heat flux $[kJ\ m^{-2}\ s^{-1}]$
ρ_a	atmospheric density $[kg\ m^{-3}]$
c_a	specific heat of moist air $[kJ\ kg^{-1}\ K^{-1}]$ (=1.013)
$e_s(T)$	saturation vapour pressure $[hPa]$ depending on average daily air temperature T [°C]
e_d	average daily vapour pressure $[hPa]$ (at dew point temperature)
r_a	aerodynamic resistance r_a $[s\ m^{-1}]$
r_c	crop canopy resistance r_c $[s\ m^{-1}]$
γ	psychrometric constant $[kPa\ K^{-1}]$ (= 0.0665 $kPa\ K^{-1}$ at 100 kPa atmospheric pressure)

The Penman-Monteith equation has gained significance mainly due to its use as the basis for calculating the standard grass reference evapotranspiration (ET_0). This standard is defined as the *'rate of evapotranspiration from a hypothetic crop with an assumed crop height of 0.12 m, a fixed canopy resistance of 70 s m^{-1} and an albedo of 0.23, closely resembling the evapotranspiration from an extensive surface of green grass of uniform height, actively growing, completely shading the ground and not short of water'*(Smith et al., 1992; Allen et al., 1998). This defines a uniquely determined specification for the calculation of daily and monthly values of this reference evapotranspiration at chosen meteorological stations world wide in a uniform way. This quantitatively-defined reference evapotranspiration is designed to replace only qualitative or unreliable methods for the estimation of the potential evapotranspiration (Smith et al., 1992; DVWK, 1996).

1.3.3.2 Resistance Factors The crop canopy resistance r_c $[s\ m^{-1}]$ is estimated from the average daily (24 hours) stomata resistance of a single leaf r_l= 100 $s\ m^{-1}$, and from the leaf area index [1] of the canopy:

$$r_c \ = \ \frac{r_l}{0.5\ LAI} \tag{28}$$

Using the relation $LAI = 24\ h_c$ and the crop height h_c =0.12 m for cut grass, a leaf area index of $LAI = 2.88$ is obtained for the grass reference crop. This yields a crop canopy resistance of $r_c \ = \ 70\ s\ m^{-1}$.

The aerodynamic resistance r_a is calculated according to Allen et al. (1989) by

$$r_a \ = \ \frac{ln(\frac{z_m - d}{z_{om}})\ ln(\frac{z_h - d}{z_{oh}})}{k^2\ v_z} \tag{29}$$

r_a	aerodynamic resistance $[s\ m^{-1}]$
z_m	height of wind speed measurements above ground in $[m]$
z_h	height of temperature and humidity measurements above ground in $[m]$
k	von Karman constant = 0.41 [1]
v_z	wind speed $[m\ s^{-1}]$ measured at height z_m above ground
d	zero plane displacement of wind profile $[m]$ (Monteith, 1981) ($d = \frac{2}{3}\ h_c = 0.08\ m$ for crop height $h_c = 0.12\ m$)
z_{om}	roughness parameter $[m]$ for momentum (Brutsaert, 1975) ($z_{om} = 0.123\ h_c = 0.015$ m for crop height $h_c = 0.12\ m$)
z_{oh}	roughness parameter $[m]$ for heat and water vapor (Brutsaert, 1975) ($z_{oh} = 0.0123\ h_c = 0.0015$ m for canopy height $h_c = 0.12\ m$)

For a standardized height for wind speed, temperature and humidity at z=2 m above ground, and a standardized crop height of 0.12 m, the aerodynamic resistance can be estimated as follows:

$$r_a \ = \ \frac{208}{v_2} \tag{30}$$

Finally the modified psychrometric constant according to (Monteith, 1965) is calculated:

$$\gamma^* = \gamma(1 + r_c/r_a) = \gamma(1 + 0.34\ v_2) \tag{31}$$

γ^*	modified psychrometric constant $[kPa\ K^{-1}]$
γ	psychrometric constant $[kPa\ K^{-1}]$
r_c	crop canopy resistance $[s\ m^{-1}]$
r_a	aerodynamic resistance $[s\ m^{-1}]$
v_2	wind velocity $[m\ s^{-1}]$ at 2 m height

1.3.3.3 Vapour Pressure Deficit and Slope of the Vapor Pressure Curve

The vapor pressure deficit $[kPa]$, i. e. the difference $e_s - e_d$ between the saturation vapour pressure e_s $[kPa]$ and the vapour pressure at dew point temperature e_d $[kPa]$, is obtained by the daily minimal und maximal air temperatures T_{min} [°C] and T_{max} [°C]:

$$e_s \;=\; \frac{1}{2}\,[\,e_a(T_{min}) \;+\; e_a(T_{max})\,], \quad \text{where} \quad e_a(T) = \;0.611\;\exp(\,\frac{17.27\,T}{237.3\;+\;T}\,) \qquad (32)$$

(Tetens, 1930) and the mean relative humidity U $[\%]$ of the day:

$$e_d \;=\; U \Big/ \left[\,\frac{50}{e_a(T_{min})} \;+\; \frac{50}{e_a(T_{max})}\,\right] \qquad (33)$$

The slope of the vapor pressure curve Δ $[kPa\;K^{-1}]$ results from Tetens (1930):

$$\Delta \;=\; \frac{4098\;e_s}{(237.3\;+\;T)^2} \qquad (34)$$

1.3.3.4 Aerodynamic Term of the Penman-Monteith Equation

The second term, the aerodynamic term $(ET_{pot}^{day})_{aer}$ $[mm\;d^{-1}]$, of the Penman-Monteith equation is given by:

$$(ET_{pot}^{day})_{aer} \;=\; \frac{86.4}{L}\;\frac{\rho_a\;c_a\;(e_s\;-\;e_d)/r_a}{\Delta\;+\;\gamma^*} \qquad (35)$$

$(ET_{pot}^{day})_{aer}$	aerodynamic term of daily potential evapotranspiration $[mm\;d^{-1}]$
L	volumetric latent heat of vaporisation $[MJ\;m^{-2}\;mm^{-1}]$, $L = \rho_w\;L^*$ ($L^* = 2.45\;MJ\;kg^{-1}$ at an average air temperature of 20 °C)
ρ_a	atmospheric density $[kg\;m^{-3}]$
ρ_w	Water density $\approx 1,0\;kg\;dm^{-3}$
c_a	specific heat of moist air $[kJ\;kg^{-1}\;K^{-1}]$
$e_s - e_d$	vapor pressure deficit $[kPa]$
r_a	aerodynamic resistance r_a $[s\;m^{-1}]$
Δ	slope of the vapor pressure curve $[kPa\;K^{-1}]$
γ^*	modified psychrometric constant $[kPa\;K^{-1}]$

From an equation to calculate the specific heat of moist air

$$c_a \;=\; \gamma\;\frac{M_w\;L^*\;10^3}{M_a\;p_a} \qquad (36)$$

c_a	specific heat of moist air $[kJ\;kg^{-1}\;K^{-1}]$
γ	psychrometric constant $[kPa\;K^{-1}]$
M_w/M_a	= $0,622$ ratio of molecular weights of water vapor to dry air [1]
L^*	specific latent heat of vaporisation $[MJ\;kg^{-1}]$
p_a	atmospheric pressure $[kPa]$

and from the ideal gas law

$$\rho_a \;=\; \frac{M_a\, p_a\, 10^3}{R\, T_v} \tag{37}$$

ρ_a	atmospheric density $[kg\ m^{-3}]$
P	atmospheric pressure $[kPa]$
R	specific gas constant = 287 $[J\ kg^{-1} K^{-1}]$
T_v	virtual temperature $[K]$
	[= 1,01 (T+273) for the daily average air temperature T]
M_a	= $28,94\ \ 10^{-3}\ kg\ mol^{-1}$ molar weight of dry air

the following aerodynamic term for the grass reference evapotranspiration is obtained (Smith et al., 1992):

$$\begin{aligned} (ET_{pot}^{day})_{aer} \;&=\; \frac{\gamma}{\Delta \,+\, \gamma^{*}}\, \frac{0.622}{p_a}\, \frac{3,486 p_a}{1,01\,(T+273)}\; 86400\, \frac{v_2}{208}\, (e_s \,-\, e_d) \\ &\approx\; \frac{\gamma}{\Delta \,+\, \gamma\,(1 + 0,34\, v_2)}\, \frac{900}{(T+273)}\, v_2\, (e_s \,-\, e_d) \end{aligned} \tag{38}$$

$(ET_{pot}^{day})_{aer}$	aerodynamic term for the daily potential evapotranspiration $[mm\ d^{-1}]$
Δ	slope of the vapor pressure curve $[kPaK^{-1}]$
γ^{*}	modified psychrometric constant $[kPa\ K^{-1}]$
γ	psychrometric constant = 0.0665 $kPa\ K^{-1}$ at 100 kPa atmospheric pressure
v_2	wind speed $[m\ s^{-1}]$ at 2 m height
T	daily average air temperature [°C]
$e_s - e_d$	vapor pressure deficit $[kPa]$

1.3.3.5 Radiation Term of the Penman-Monteith Equation The first term of the Penman-Monteith is the radiation term $(ET_{pot}^{day})_{rad}$ $[mm\ d^{-1}]$. For the grass reference evapotranspiration it is given by

$$(ET_{pot}^{day})_{rad} \;=\frac{1}{L}\, \frac{\Delta\,(Rn \,-\, G)}{\Delta \,+\, \gamma^{*}} \;=\; 0.408\, \frac{\Delta\,(Rn \,-\, G)}{\Delta \,+\, \gamma\,(1 \,+\, 0.34\, v_2)} \tag{39}$$

$(ET_{pot}^{day})_{rad}$	radiation term for the daily potential evapotranspiration $[mm\ d^{-1}]$
L	volumetric latent heat of vaporisation $[MJ\ m^{-2}\ mm^{-1}]$, $L = \rho_w\ L^{*}$
	($L^{*} = 2.45\ MJ\ kg^{-1}$ at an average air temperature of 20 °C)
Δ	slope of the vapour pressure curve $[kPa\ K^{-1}]$
Rn	net radiation at the soil surface $[MJ\ m^{-2}\ d^{-1}]$
G	soil heat flux across the soil surface $[MJ\ m^{-2}\ d^{-1}]$
γ	modified psychrometric constant $[kPa\ K^{-1}]$ with γ = 0.0665 $kPa\ K^{-1}$
v_2	wind speed $[m\ s^{-1}]$ at 2 m height

Thereby, the net radiation $Rn\ [MJ\ m^{-2}\ d^{-1}]$ is given by the difference between the net incoming shortwave radiation $Rn_s\ [MJ\ m^{-2}\ d^{-1}]$ and the net outgoing longwave radiation $Rn_l\ [MJ\ m^{-2}\ d^{-1}]$, where the net shortwave radiation Rn_s can be calculated from the measured daily cumulative solar radiation $R_g\ [MJ\ m^{-2}\ d^{-1}]$, if the albedo α_c of the canopy is known (e.g. α_g=0.23 for grass):

$$Rn \;=\; Rn_s - Rn_l \;= (1-\alpha_g)\; R_g - Rn_l \tag{40}$$

The net outgoing longwave radiation $Rn_l\ [MJ\ m^{-2}\ d^{-1}]$ is the difference between the outgoing thermal radiation emitted by the vegetation and soil into the atmosphere and the incoming thermal radiation emitted by the atmosphere and cloud cover to the earth surface:

$$Rn_l \;=\; f\;(\epsilon_a \;-\; \epsilon_{vs})\;\sigma\;(T+273.15)^4 \tag{41}$$

Rn_l	net outgoing longwave radiation $[MJ\ m^{-2}\ d^{-1}]$
f	cloud cover factor [1]
ϵ_a	effective emissivity of the atmosphere [1]
ϵ_{vs}	emissivity by vegetation and soil [1]
σ	Stefan- Boltzmann constant = 4.9 $10^{-9}\ MJ\ m^{-2}\ K^{-4}\ d^{-1}$
T	daily average air temperature [°C]

The net emissivity $\epsilon_a - \epsilon_{vs}$ [1] can be estimated using the equation of Brunt (1932), see also Jensen et al. (1990), from the vapor pressure at dew point temperature e_d [kPa]:

$$\epsilon_a \;-\; \epsilon_{vs} \;=\; (\;0.34\;-\;0.14\;\sqrt{e_d}\;) \tag{42}$$

The cloud cover factor f [1] can be determined from the relative sunshine fraction, i.e. the ratio n/N between the duration of bright sunshine [h] and the total daylength [h]:

$$f \;=\; 0.9\,\frac{n}{N} \;+\; 0.1 \tag{43}$$

Summarizing, for the net longwave radiation $Rn_l\ [MJ\ m^{-2}\ d^{-1}]$ results:

$$\begin{aligned} Rn_l \;&=\; (0.9\,\tfrac{n}{N}\;+\;0.1)\,(0.34\;-\;0.14\,\sqrt{e_d})\;\;\sigma\;\;\tfrac{1}{2}\,(T_{min}^4\;+\;T_{max}^4) \\ &=\; 2.45\;10^{-9}\,(0.9\,\tfrac{n}{N}\;+\;0.1)\,(0.34\;-\;0.14\,\sqrt{e_d})\,(T_{min}^4\;+\;T_{max}^4) \end{aligned} \tag{44}$$

Rn_l	net outgoing longwave radiation $[MJ\ m^{-2}\ d^{-1}]$
n	daily duration of bright sunshine [h]
N	total day length [h]
e_d	atmospheric pressure $[kPa]$
σ	Stefan-Boltzmann constant = 4.9 $10^{-9}\ MJ\ m^{-2}\ K^{-4}\ d^{-1}$
T_{min}, T_{max}	minimal and maximal air temperature of the day $[K]$

If no measured data on the sunshine duration n are available, it can be estimated from the measured daily solar radiation R_g $[MJ\ m^{-2}\ d^{-1}]$ by:

$$n \ = \ N\,(R_g/R_a \ - \ A)/B \tag{45}$$

n	sunshine duration [h]
N	total daylength [h]
R_{sol}	daily solar radiation $[MJ\ m^{-2}\ d^{-1}]$
R_a	extraterrestrial radiation $[MJ\ m^{-2}\ d^{-1}]$
A, B	constants $A = 0.25$ and $B = 0.5$for an average climate (Smith et al., 1992),
	or $A = 0,35$ and $B = 0,55$ for the whole region of Germany (DVWK, 1996).

The extraterrestrial radiation R_a $[MJ\ m^{-2}\ d^{-1}]$ and the total daylength N $[h]$ of the day can be estimated from geometrical considerations on the position of the sun (Duffie and Beckman, 1980) :

$$R_a \quad = \quad \frac{24 \cdot 60}{\pi}\, G_{sc}\, d_r\, (\omega_s \ \sin\phi\ \sin\delta \ + \ \cos\phi\ \cos\delta\ \sin\omega_s) \tag{46}$$

$$N \quad = \quad \frac{24}{\pi}\,\omega_s \ = \ 7.64\,\omega_s \tag{47}$$

R_a	extraterrestrial radiation $[MJ\ m^{-2}\ d^{-1}]$
G_{sc}	solar constant =0.0820 $MJ\ m^{-2}\ min^{-1}$
d_r	relative distance Earth-Sun [1]
	[$d_r = 1 + 0.033\ \cos(\frac{2\pi}{365}J) = 1 + 0.033\ \cos(0.0172J)$]
δ	solar declination [rad]
	[$\delta = 0.409\ \sin(\frac{2\pi}{365}J - 1.39) = 0.409\ \sin(0.0172J - 1.39)$]
ϕ	latitude [rad]
ω_s	sunset hour angle [rad]
	[$\omega_s = \arccos(-\tan\phi\ \tan\delta)$]
J	number of the day in the year (1,...,365)
N	total daylength $[h]$

1.3.3.6 Soil Heat Flux Estimation for the Grass Reference Evapotranspiration For the determination of the grass reference evapotranspiration also an estimation of the soil heat flux G $[MJ\ m^{-2}\ d^{-1}]$ is needed. According to Wright and Jensen (1972) this can be done in an approximative way for an effective soil depth of 0.18 m as follows:

$$G \ = \ 0.38\,(T_{day,n} \ - \ T_{day,n-1}) \tag{48}$$

G	soil heat flux into the soil $[MJ\ m^{-2}\ d^{-1}]$
$T_{day,n}$	average air temperature on the actual day [°C]
$T_{day,n-1}$	average air temperature on the preceding day [°C]

1.3.3.7 Grass Reference Evapotranspiration (FAO) By summing up the aerodynamic and the radiation term, i.e. equation (38) and equation (39), the Penman-Monteith equation for the standardized determination of the grass reference evapotranspiration rate $(ET_{pot}^{day})_0$ $[mm\ d^{-1}]$ results, which is independent from water supply and from crop canopy state:

$$(ET_{pot}^{day})_0 \ = \ \frac{0.408\ \Delta\ (Rn - G)\ +\ \gamma\ \dfrac{900}{T + 273}\ v_2\ (e_a - e_d)}{\Delta\ +\ \gamma\ (1 + 0.34\ v_2)} \tag{49}$$

$(ET_{pot}^{day})_0$	daily standard grass reference evapotranspiration rate $[mm\ d^{-1}]$
Δ	slope of the vapor pressure curve $[kPa\ K^{-1}]$
Rn	net radiation at the crop surface $[MJ\ m^{-2}\ d^{-1}]$
G	soil heat flux across the soil surface $[MJ\ m^{-2}\ d^{-1}]$
γ	psychrometric constant = 0.0665 $kPa\ K^{-1}$ at 100 kPa atm. pressure
T	daily average air temperature [°C]
v_2	wind speed $[m\ s^{-1}]$ at 2 m height
$e_s - e_d$	vapour pressure deficit $[kPa]$

1.3.3.8 Crop coefficients for different crops The grass reference evapotranspiration $(ET_{pot}^{day})_0$ provides a standard to which evapotranspiration in different periods of the year and from other crops can be related. This relation is expressed by crop coefficients which basically are the ratios of the crop evapotranspiration to the reference evapotranspiration. Consequently, the crop coefficient represents the integration of the major effects that distinguish the evapotranspiration of the crop from the reference (Allen, 2000). In the FAO-56 report (Allen et al., 1998) and in Allen (2000) the relation to the standard reference is used to define an upper limit on the actual evaporation and actual transpiration from any cropped surface. This upper limit corresponds to the potential evapotranspiration from a wet soil after complete wetting of the soil surface by precipitation or irrigation. This potential evapotranspiration is determined by the maximal crop coefficient $K_{c,max}$ for the respective crop depending on crop height, wind speed and relative humidity:

$$(ET_{pot}^{day})_c \ = \ K_{c,max}\ (ET_{pot}^{day})_0 \tag{50}$$

$(ET_{pot}^{day})_c$	daily potential evapotranspiration rate of the crop $[mm\ d^{-1}]$
$(ET_{pot}^{day})_0$	daily potential grass reference evapotranspiration rate $[mm\ d^{-1}]$
$K_{c,max}$	maximal crop coefficient [1]

where

$$K_{c,max} = max(\{\kappa + [0.04(v_2 - 2) - 0.004(U_{min} - 45)](\frac{h}{3})^{0.3}\}, \{K_{cb} + 0.05\}) \quad (51)$$

$$\kappa = \begin{cases} 1.2 & \text{for } \tau \geq 3\ d \\ 1.1 & \text{else} \end{cases} \quad (52)$$

$K_{c,max}$	maximal crop coefficient [1]
K_{cb}	basal crop coefficient [1]
v_2	wind speed $[m\ s^{-1}]$ in 2 m height
U_{min}	daily minimal relative air humidity $[\%]$
h	average crop canopy height $[m]$
τ	time distance between two precipitation or irrigation events $[d]$

The daily minimal relative air humidity U_{min} $[\%]$ is estimated by the ratio of the atmospheric pressures $e_a(T_{min})/e_a(T_{max})$ at the minimal and the maximal air temperature of the day T_{min} $[°C]$, respectively, T_{max} $[°C]$:

$$U_{min} = 100 \left[\exp(\frac{17.27\ T_{min}}{237.3\ +\ T_{min}}) \middle/ \exp(\frac{17.27\ T_{max}}{237.3\ +\ T_{max}}) \right] \quad (53)$$

The daily potential evaporation EV_{pot}^{day} $[mm\ d^{-1}]$ and the daily potential transpiration TR_{pot}^{day} $[mm\ d^{-1}]$ are distributed by the use of the plant specific soil cover factor f_{plcv} [1] and, by considering the daily actual evaporation of the interception storage EI_{act}^{day} $[mm\ d^{-1}]$ as follows:

$$EV_{pot}^{day} = min\{(K_{c,max} - K_{cb}), (1 - f_{plcv})K_{c,max}\}\ (ET_{pot}^{day})_0 \quad (54)$$

$$TR_{pot}^{day} = max\{K_{cb}, f_{plcv}K_{c,max}\}\ (ET_{pot}^{day})_0\ -\ EI_{act}^{day} \quad (55)$$

To determine the basal crop coefficient K_{cb} [1] four different crop growth stage periods are distinguished: the initial, the development, the midseason and the late season period. In correspondence to leaf area index which increases respectively stays constant in the first three periods and decreases in the last, the basal crop coefficient K_{cb} [1] is constant during the initial and midseason periods, increases in the development period and decreases in the late season. Hence, for the first three periods K_{cb} [1] is given by:

$$K_{cb} = \begin{cases} K_{cb,ini} & \text{for } 0 \leq t < t_{ini} \\ K_{cb,ini} + (K_{cb,mid} - K_{cb,ini})\ \dfrac{t - t_{ini}}{t_{dev} - t_{ini}} & \text{for } t_{ini} \leq t < t_{dev} \\ K_{cb,mid} & \text{for } t_{dev} \leq t < t_{mid} \end{cases} \quad (56)$$

and for the late season period $(\, t_{mid} \leq t \leq t_{end} \,)$ by:

$$K_{cb} \;=\; K_{cb,mid} \;+\; (K_{cb,end} - K_{cb,mid}) \, \frac{t - t_{mid}}{t_{end} - t_{mid}} \tag{57}$$

K_{cb}	basal crop coefficient $[1]$
$K_{cb,ini}$	basal crop coefficient during the initial period $[1]$
$K_{cb,mid}$	basal crop coefficient during the midseason period $[1]$
$K_{cb,end}$	basal crop coefficient during the late season period $[1]$
t	time $[d]$
t_{ini}	end of the initial period $[d]$
t_{dev}	end of the development period $[d]$
t_{mid}	end of the midseason period $[d]$
t_{end}	end (and duration) of the total period $[d]$

Table 2: basal crop coefficients (Allen et al., 1998)

	t_{ini}	t_{dev}	t_{mid}	t_{end}	$K_{cb,ini}$	$K_{cb,mid}$	$K_{cb,end}$
PO	30	65	115	145	0.15	1.10	0.65
SF	25	60	105	130	0.15	1.10	0.25
SB	45	120	200	230	0.15	1.15	0.90
WC	30	170	210	240	0.15	1.10	0.15
SC	40	70	110	130	0.15	1.10	0.15
MA	30	70	120	150	0.15	1.15	0.15

PO	potato	SF	sunflower	SB	sugar beet (winter)
WC	winter cereals	SC	summer cereals	MA	maize (grain)

These values for the basal crop coefficients $K_{cb,mid}$ and $K_{cb,end}$ are adjusted, if the minimal relative air humidity during the day U_{min} is different from 45% and the wind speed in 2 m height v_2 is not 2.0 m s^{-1} according to (Allen, 2000):

$$K_{cb,mid} \;=\; K_{cb,mid\;(table)} \;+\; [0.04\;(v_2 - 2) - 0.004\;(U_{min} - 45)](\frac{h}{3})^{0.3} \tag{58}$$

$$K_{cb,end} \;=\; K_{cb,end\;(table)} \;+\; [0.04\;(v_2 - 2) - 0.004\;(U_{min} - 45)](\frac{h}{3})^{0.3} \tag{59}$$

1.3.3.9 Direct Consideration of Crop Canopies Instead of calculating one reference evapotranspiration and using crop coefficients to convert to potential evaporation and transpiration, the Penman-Monteith equation can be evaluated directly using different resistance factors, crop heights and albedos for different crops, e.g. Droogers (2000).

First the daily potential evaporation of a wet, bare soil $(EV_{pot}^{day})_0$ $[mm\ d^{-1}]$ and the daily potential transpiration $(TR_{pot}^{day})_0$ $[mm\ d^{-1}]$ of a crop canopy completely covering the soil is determined by using the Penman-Monteith equation:

$$(EV_{pot}^{day})_0 = \frac{1}{L}\,\frac{\Delta\,[(1-\alpha_s)\,R_g - Rn_l\ -\ G]\ +\ \rho_a\,c_a\,(e_s\ -\ e_d)/r_{as}}{\Delta\ +\ \gamma} \tag{60}$$

$$(TR_{pot}^{day})_0 = \frac{1}{L}\,\frac{\Delta\,[(1-\alpha_c)\,R_g - Rn_l\ -\ G]\ +\ \rho_a\,c_a\,(e_s\ -\ e_d)/r_{ac}}{\Delta\ +\ \gamma\,(1\ +\ r_c/r_{ac})}\ -\ EI_{act}^{day} \tag{61}$$

$(EV_{pot}^{day})_0$	daily potential evapotranspiration of a wet, bare soil $[mm\ d^{-1}]$
$(TR_{pot}^{day})_0$	daily pot. transpiration of a wet crop canopy completely covering the soil $[mm\ d^{-1}]$
EI_{act}^{day}	actual evaporation of the interception storage $[mm\ d^{-1}]$
L	volumetric latent heat of vaporization $[MJ\ m^{-2}\ mm^{-1}]$
Δ	slope of the vapor pressure curve $[hPa\ K^{-1}]$
R_g	daily cumulative solar radiation $[MJ\ m^{-2}\ d^{-1}]$
α_s, α_c	soil albedo, respectively crop albedo [1]
Rn_l	net outgoing longwave radiation $[MJ\ m^{-2}\ d^{-1}]$
G	soil heat flux $[MJ\ m^{-2}\ d^{-1}]$
ρ_a	atmospheric density $[kg\ m^{-3}]$
c_a	specific heat of moist air $[MJ\ kg^{-1}\ K^{-1}]$ (=1.013)
$e_s - e_d$	vapor pressure deficit $[kPa]$
r_{as}, r_{as}	aerodynamic resistances for soil r_{as} $[s\ m^{-1}]$ and crop r_{ac} $[d\ m^{-1}]$
r_c	crop canopy resistance r_c $[d\ m^{-1}]$
γ	psychrometric constant $[kPa\ K^{-1}]$ (= 0.0665 $kPa\ K^{-1}$ at 100 kPa atmospheric pressure)

Second, the soil cover fraction by plants f_{plcv} [1] is used to distribute the above rates into the daily potential evaporation EV_{pot}^{day} $[mm\ d^{-1}]$ and transpiration TR_{pot}^{day} $[mm\ d^{-1}]$:

$$EV_{pot}^{day} = (1-f_{plcv})\,(EV_{pot}^{day})_0 \tag{62}$$

$$TR_{pot}^{day} = f_{plcv}\,(TR_{pot}^{day})_0 \tag{63}$$

where the soil cover fraction can be obtained from the leaf area index LAI [1] of the canopy as follows:

$$f_{plcv}\ =\ \exp(0.45\ LAI) \tag{64}$$

1.3.4 Potential Evapotranspiration - Haude (VDI) Method

For Germany Haude (1955) was the first who proposed an approach based on the method of Dalton to calculate the mean daily potential evapotranspiration $[mm\ d^{-1}]$ (DVWK, 1996). As input data, the air temperature T [°C] in 2 m height (10 min mean at 13:30 GMT), the relative air humidity U $[\%]$ (10 min mean at 13:30 GMT) and monthly crop factors f_{Haude} ('Haude factors') are required. The *Haude formula* is given by:

$$ET_{pot}^{day} \ = \ f_{Haude} \ \ (\ e_s(T) \ - \ e_d \ )_{13:30} \tag{65}$$

ET_{pot}^{day}	daily potential evapotranspiration $[mm\ d^{-1}]$
$e_s(T)$	saturation vapour pressure $[hPa]$ at 13:30 GMT depending on the air temperature T [°C] at 13:30 GMT
e_d	actual vapour pressure $[hPa]$ at 13:30 GMT)
f_{Haude}	Haude factor $[mm\ d^{-1}\ hPa^{-1}]$ for the specific month and crop

Similar as for the Penman equation the vapour pressure deficit $[hPa]$ at 13:30 Uhr GMT is estimated using the relative air humidity U $[\%]$ and air temperature T [°C] at 13:30 GMT:

$$(\ e_s(T) \ - \ e_d \ )_{13:30} \ = \ (1 \ - \ \frac{U}{100}) \ 6.11 \ \ \exp(\ \frac{17.62\,T}{243.12 \ + \ T} \ ) \tag{66}$$

Generally, the Haude method is not accurate enough to estimate the potential evapotranspiration for a single day. But, for calculating monthly and yearly averages and for a regional survey, the method is proven to be reliable (DVWK, 1996).

Table 3: Haude Factors $[mm\ d^{-1}\ hPa^{-1}]$ VDI (1993)

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
SF	0.08	0.04	0.14	0.35	0.39	0.34	0.31	0.25	0.20	0.13	0.07	0.05
BF	0.01	0.00	0.04	0.10	0.23	0.28	0.32	0.26	0.17	0.10	0.01	0.00
GR	0.20	0.20	0.22	0.24	0.29	0.29	0.28	0.26	0.23	0.20	0.20	0.20
PA	0.20	0.20	0.25	0.29	0.29	0.28	0.26	0.25	0.23	0.22	0.20	0.20
MA	0.11	0.11	0.11	0.17	0.21	0.24	0.25	0.26	0.21	0.18	0.11	0.11
SB	0.11	0.11	0.11	0.15	0.23	0.30	0.37	0.33	0.26	0.20	0.11	0.11
WW	0.11	0.11	0.17	0.24	0.33	0.41	0.37	0.28	0.15	0.11	0.11	0.11
WB	0.11	0.11	0.17	0.24	0.37	0.38	0.32	0.22	0.15	0.11	0.11	0.11
OA	0.11	0.11	0.11	0.15	0.34	0.44	0.45	0.30	0.19	0.11	0.11	0.11
RY	0.11	0.11	0.17	0.23	0.30	0.36	0.36	0.27	0.15	0.11	0.11	0.11

SF	spruce forest	BF	beech forest	GR	grass	PA	pasture	MA	maize
SB	sugar beet	WW	winter wheat	WB	winter barley	OA	oat	RY	rye

1.3.5 Potential Evapotranspiration - Ritchie (CERES) Method

To calculate soil evaporation and plant transpiration according to the method of Ritchie (1972) data on the average daily air temperature T_{day} $[°C]$, the soil albedo [1], the plant albedo [1] and the solar radiation R_{sol} $[MJ\ m^{-2}\ d^{-1}]$ are used. The mean daily air temperature is estimated from the maximal T_{max} $[°C]$ and the minimal T_{min} $[°C]$ daily air temperature by:

$$T_{day} = 0.6\, T_{max} \ +\ 0.4\, T_{min} \tag{67}$$

The weighting between T_{max} and T_{min} considers the decrease of transpiration during the night, when the plant stomata are closed. The total albedo $\alpha_g[1]$ of soil and plants is calculated from the soil albedo α_s [1] and the leaf area index LAI [1] depending on the time of crop emergence t_{em} $[d]$, begin t_{bcf} $[d]$ and end t_{ecf} $[d]$ of the grain filling phase and the time of physiological maturity t_m $[d]$:

$$\alpha_g = \begin{cases} \alpha_s & \text{for } t \le t_{bcf} \\ 0.23\ -\ (0.23\ -\ \alpha_s)\ \exp(-0.75\, LAI) & \text{for } t_{bcf} < t \le t_{ecf} \\ 0.23\ +\ (LAI\ -\ 4)^2/160 & \text{for } t_{ecf} < t \le t_m \end{cases} \tag{68}$$

The equilibrium potential evapotranspiration $ET_{pot,eq}$ $[mm\ d^{-1}]$ occurs at high air humidity, when it is in equilibrium with the soil water of the soil surface. It is estimated by:

$$ET_{pot,eq} = R_g\ (4.88\ 10^{-3}\ -\ 4.37\ 10^{-3}\ \alpha_g)\ (29.0\ +\ T_{day}) \tag{69}$$

α_g	albedo [1]
R_g	cumulative daily solar radiation $[MJ\ m^{-2}]$
T_{day}	mean daily air temperature $[°C]$

The daily potential evapotranspiration ET^{pot}_{day} $[mm]$ is then calculated as the equilibrium potential evapotranspiration $ET_{pot,eq}$ multiplied by 1.1 to account for the effects of unsaturated air. This multiplier is increased (>1.1) to allow for advection when the maximum air temperature of the day T_{max} $[°C]$ is greater than 35°C. It is reduced for temperatures below 5°C to account for the influence of cold temperatures on stomatal closure:

$$ET^{pot}_{day} = \begin{cases} ET_{pot,eq}\ 0.01\ \exp[0.18\ (T_{max}\ +\ 20.0)] & \text{for } T_{max} < 5.0°C \\ ET_{pot,eq}\ 1.1 & \text{for } 5.0°C \le T_{max} < 35.0°C \\ ET_{pot,eq}\ [(T_{max}\ -\ 24.0)\ 0.05\ +\ 1.1] & \text{for } 35.0°C < T_{max} \end{cases} \tag{70}$$

Finally the daily potential soil evaporation EV^{pot}_{day} $[mm]$ depending on the leaf area index LAI [1] results from:

$$EV^{pot}_{day} = \begin{cases} ET^{pot}_{day}\ (1.0\ - 0.43\, LAI) & \text{for } LAI\ <\ 1.0 \\ ET^{pot}_{day}\ \exp(-0.4\, LAI) & \text{for } 1.0 \le LAI \end{cases} \tag{71}$$

1.3.6 Interception Models

The quantification of all relevant water fluxes in terrestrial ecosystems often also includes the determination of interception and related water fluxes. This means we need to determine storage and evaporation of water that is wetting plant surfaces during and after precipitation or irrigation. To calculate the net-precipitation, i.e. the part of the gross-precipitation which reaches the soil, different interception models have been developed that can simulate water storage caused by canopy interception as well as interception evaporation, throughfall and interception drainage including stem flow.

For forest systems one of the well known models is the Rutter model (Rutter et al., 1971; Bouten et al., 1996; Klaassen et al., 1998) which was simplified by Gash (1979), see also Gash et al. (1995); Valente et al. (1997). For agricultural systems von Hoyningen-Huene (1981) and Braden (1985) investigated the interception of precipitaton in different crop canopies and developed a simple interception model for agricultural crops.

Rutter Model The model of Rutter calculates the amount of water S $[mm]$ that is wetting the plant surfaces and thus is temporarily stored by the canopy by applying a time-continuous dynamical non-stationary modelling approach. Besides the water storage S $[mm]$ this approach also considers the evaporation rate E $[mm\ d^{-1}]$ and the drainage D $[mm\ d^{-1}]$ from the wetted plant surfaces, assuming the drainage to consist of both canopy drip and stem flow:

$$\frac{dS}{dt} = (1-a)\,R \,-\, D \,-\, E \tag{72}$$

$$D = \begin{cases} 0 & \text{for} \quad S < c \\ b\,(S \,-\, c) & \text{for} \quad S \geq c \end{cases} \tag{73}$$

$$E = \begin{cases} d\,ET_{pot}\,S/c & \text{for} \quad S < c \\ ET_{wet} & \text{for} \quad S \geq c \end{cases} \tag{74}$$

S	water storage due to interception $[mm]$
R	precipitation rate $[mm\ d^{-1}]$ given by $R = dP/dt$
D	drainage from canopy to soil $[mm\ d^{-1}]$ (canopy drip plus stem flow)
E	interception evaporation rate $[mm\ d^{-1}]$
P	(gross-)precipitation $[mm]$
a	fraction of throughfall $[1]$ (empirical parameter)
b	fraction of drainage $[1]$ (empirical parameter)
c	canopy storage capacity of interception (empirical parameter)
d	evaporation coefficient (empirical parameter)
ET_{pot}	potential evapotranspiration rate $[mm\ d^{-1}]$
ET_{wet}	potential evapotranspiration rate $[mm\ d^{-1}]$ during precipitation, e.g. calculated according to Penman-Monteith (FAO) with zero stomatal resistance ($r_s = 0$)

The empirical parameters a, b, c, d can be estimated, for example, by fitting the model to measured data of net-precipitation possibly available for a certain period. The simulated or predicted net-precipitation rate then results by adding the simulated rates of throughfall and drainage (canopy drip plus stem flow) that reaches the soil.

Gash Model Based on the model of Rutter, Gash developed a time-discrete dynamical interception model. For this purpose precipitation is conceived as a series of single precipitation events, where each event consists itself of three different phases, i.e.

- of the wetting phase, from the onset of the precipitation event until the saturation of the interception storage capacity of the canopy,
- of the saturation phase, i.e. when the interception storage capacity of the canopy is saturated during the precipitation event and
- of the drying phase, from the end of the precipitation event until the total drying of the plant surfaces of the canopy.

The interception amount I $[mm]$ during a precipitation event of duration $\Delta t = [t_0, t_e]$ represented by the time interval is given by the sum of the amount of water S_e $[mm]$ stored at the plant surfaces during this time and the amount of water E_e $[mm]$ that already evaporated from this water storage

$$I \;=\; S_e \;+\; E_e \;=\; \int_{\Delta t} \frac{dS}{dt}\, dt \;+\; \int_{\Delta t} E\, dt \tag{75}$$

assuming a constant evaporation rate E $[mm\ d^{-1}]$ for the evaporation from the plant surfaces. According to the model of Rutter, equation (72), we get:

$$S_e \;=\; \int_{\Delta t} \frac{dS}{dt}\, dt \;=\; \int_{\Delta t} (1-a)R - D - E\, dt \;=\; (1-a)P - \int_{\Delta t} D\, dt - E_e \;=\; P - E_e - Q \tag{76}$$

where the net-precipitation Q $[mm]$ is given by the sum of throughfall, canopy drip and stem flow:

$$Q \;=\; aP \;+\; \int_{\Delta t} D\, dt \tag{77}$$

The interception then results from:

$$I \;=\; S_e \;+\; E_e \;=\; (P \;-\; E_e \;-\; Q) \;+\; E_e \;=\; P \;-\; Q \tag{78}$$

To distinguish between wetting and saturation phase the amount of precipitation is calculated that is needed to reach the canopy interception capacity. This has to include the calculation of the evaporation which occurs during the process of saturation.

From the model of Rutter then follows, that during the filling of the interception storage capacity, i.e. as long as $S \; < \; c$, no drainage occurs, i.e. it is $D \; = \; 0$, and that the following equation holds, if interception evaporation during filling is assumed to be constant and given by the term $E \; (S/c)$ for $d = 1$ and $E = ET_{wet}$:

$$\frac{dS}{dt} \; = \; (1-a) \, R \; - \; E \; (S/c) \tag{79}$$

By integration with respect to time results, if also a constant precipitation rate R is assumed during filling:

$$S \; = \; (1-a) \frac{R \, c}{E} \; [1 - \exp(-E t_s/c] \tag{80}$$

From this the time $t_s \; d$ when the interception storage capacity is reached, i.e. $S = c$, can be calculated:

$$t_s \; = \; - \, c/E \; \log[1 - (E/R)/(1-a)] \tag{81}$$

Finally one gets the precipitation amount $P_s \; [mm]$ necessary to fill the interception storage capacity:

$$P_s \; = \; R \, t_s \; = \; - \, \frac{R \, c}{E} \; \log[1 - (E/R)/(1-a)] \tag{82}$$

During the wetting phase as long as the interception water storage capacity is not completely filled and the precipitation amount P is still below P_s, there is no canopy drip and no stem flow, i.e. there is zero drainage $D = 0$. Therefore, if $P \; < \; P_s$, the interception $I \; [mm]$ is given by:

$$I \; = \; (1-a) \, P \tag{83}$$

During the saturation phase, when the interception storage capacity is saturated, i.e. $S_e = c$, then S_e is constant and the supplementary interception is given by:

$$\frac{dI}{dP} \; = \; \frac{dS_e}{dP} \; + \; \frac{dE_e}{dP} \; = \; \frac{dE_e}{dP} \; = \; 1/R \; \frac{d}{dt}(\int E \; dt) \; = \; E/R \tag{84}$$

Therefore, for the case $P \; \geq \; P_s$, the interception $I \; [mm]$ is obtained by further assuming a constant ratio between E and R during precipitation (Gash, 1979), using equation (83) and integrating equation (84):

$$I \; = \; (1-a) \, P_s \; + \; (E/R) \; \; (P \; - \; P_s) \tag{85}$$

For the application of the Gash-Model the empirical interception parameters a, c and E/R are needed as input. As for the Rutter-model they may be estimated by using measured data of throughfall or net-precipitation. Alternatively, parameter values can be chosen from corresponding tables depending on tree species and tree density (de Vries et al., 2001).

von Hoyningen-Huene and Braden Model Although the significance of interception during precipitation for the determination of the water balance was well known from forest hydrologic investigations, interception in agricultural crops was at first underestimated and considered to be negligible. One reason for this might have been the relatively high error of precipitation measurement e.g. due to the impact of wind and evaporation. Therefore, precipitation amounts often have been underestimated leading partly to a compensation of the lack of water in the water balance, which occurred by ignoring interception (von Hoyningen-Huene, 1981; von Hoyningen-Huene and Nasdalack, 1985).

In contrary to forestal crops, interception evaporation during precipitation can be neglected for agricultural crops. Therefore, for agricultural crops interception can be calculated by using a simple saturation approach, for which only one empirical interception parameter has to be determined and used as model input (Braden, 1985):

$$I^{day} \;=\; a\, f_{LAI} \; \left[1 - \frac{a\, f_{LAI}}{a\, f_{LAI} + f_{plcv}\, P^{day}_{grs}} \right] \tag{86}$$

I^{day}	daily interception $[mm]$ (i.e. the amount of water intercepted from precipitation during one day)
P^{day}_{grs}	daily (gross-)precipitation $[mm]$
a	plant specific interception storage capacity per leaf area $[mm]$ (empirical parameter). For an average canopy a value of $a = 2,5\,mm$ is assumed
f_{LAI}	leaf area index [1]
f_{plcv}	plant cover factor [1] ($\approx\; f_{LAI}/3$)

For increasing values of daily (gross-)precipitation the calculated daily interception approximates the saturation value $a\; f_{LAI}\; [mm]$, which is the product of the empirical parameter $a\; [mm]$ and the leaf area index $f_{LAI}\; [1]$. If no precipitation falls, then also no interception occurs, hence the interception curve given by equation (86) passes through the origin (zero-point). There, the curve attains its maximal slope, prescribed by the plant cover fraction $f_{plcv}\; [1]$.

1.4 Darcy-Buckingham Model

1.4.1 Equations of Soil Water Flow Dynamics

1.4.1.1 Darcy's Law During investigations of the fountains in the city of Dijon, France, Darcy (1856) established empirically a linear relationship between the hydraulic gradient $\Delta H / \Delta z$ [1] and the volumetric water flux q_w $[mm\ d^{-1}]$ through a vertical saturated sand column:

$$q_w \ = \ -K_{sat} \, \frac{\Delta H}{\Delta z} \tag{87}$$

The volumetric water flux q_w $[mm\ d^{-1}]$ is the volume of water flowing per unit of time through a unit area perpendicular to the direction of flow. ΔH $[mm]$ is the height difference between the upper end of the water column resting on the sand surface and the lower end of the soil column, where the water flows out. Δz $[mm]$ is the sand column length and K_{sat} $[mm\ d^{-1}]$ is the saturated hydraulic conductivity depending on the porous medium, in this case the type of sand.

1.4.1.2 Darcy-Buckingham Law To describe water flow through unsaturated soils Darcy's law, equation (87), was extended to a more general form by Buckingham (1907). The coefficient K, the hydraulic conductivity, now depends on the water content θ, a quantity which changes with flowing. Since in most cases this dependency is nonlinear, the more general Darcy-Buckingham law is a nonlinear flux law:

$$q_w \ = -K(\theta) \, \frac{dH}{dz} \tag{88}$$

q_w	volumetric water flux $[mm\ d^{-1}]$
$K(\theta)$	unsaturated hydraulic conductivity $[mm\ d^{-1}]$
θ	volumetric water content $[mm^3\ mm^{-3}]$
dH/dz	hydraulic gradient [1]
H	soil water potential [mm] (expressed in potential energy of soil water per unit weight of water)
z	soil depth $[mm]$

Notation: The water potential ψ_w is defined as an energy density, i.e. as the potential energy of soil water per unit volume of water. ψ_w thus has the dimension of pressure $[Pa]$. Instead of relating the soil's water potential energy to the volume of water, it is often determined per weight of water and the water potential is expressed as an equivalent in height $H = \psi_w / (\rho_w \ g)$. H is then called hydraulic head and has the dimension of length $[mm]$.

In the following it is assumed that the direction of the depth z is downward positive, i.e. that z points to the centre of Earth. Additionally, the reference height z_0 of a reservoir of pure and free water, which gives the reference state for soil water potential measurements, is assumed to be the height of the soil surface, i.e. $z_0 = 0$. Furthermore, by convention, the gravitational potential at a position z above the reference height z_0 is higher than at the reference point itself. Therefore, the gravitational potential ψ_g $[Pa]$ at point z $[mm]$ is given by

$$\psi_g = -\rho_w\, g\, (z - z_0) = -\rho_w\, g\, z \tag{89}$$

where $\rho_w \approx 1.0\ kg\ dm^{-3}$ stands for the density of water and $g = 9.81\ m\ s^{-2}$ for the acceleration of gravity. Neglecting the osmotic potential the water potential or hydraulic potential of the soil (as energy density) ψ_w $[kPa]$ is the sum of the matric potential ψ_m $[Pa]$ and the gravitational potential ψ_g $[Pa]$:

$$\psi_w = \psi_m + \psi_g = \psi_m - \rho_w\, g\, z \tag{90}$$

Expressing the water potential as energy per unit weight of water, i.e. by the hydraulic head $H = \psi_w/(\rho_w\ g)$ and the matric head $h = \psi_m/(\rho_w\ g)$, one gets

$$H = h - z \tag{91}$$

1.4.1.3 Mass Balance Equation Assuming that as a first approximation the soil can be considered as a rigid porous medium, the mass balance equation for soil water is given by

$$\frac{\partial \theta}{\partial t} + \frac{\partial q_w}{\partial z} + S_w = 0 \tag{92}$$

where $S_w = S_w(t, z, \theta(h))$ $[mm\ mm^{-1}\ d^{-1}]$ denotes the sink term representing the root water uptake rate.

1.4.1.4 Richards Equation Inserting q_w from the Darcy-Buckingham equation (88) into the mass balance equation (92) yields the Richards equation in it's mixed form:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[\, K(\theta(h))\, (\, \frac{\partial h}{\partial z} - 1\,)\,] - S_w(t, z, \theta(h)) \tag{93}$$

where $\theta(h)$ [1] is called water retention function describing the volumetric soil water content as function of the matric potential. Applying the chain rule of differentiation to $\partial\theta/\partial t$ the head form of the Richards equation is obtained:

$$C(h)\, \frac{\partial h}{\partial t} = \frac{\partial}{\partial z}[\, K(h)\, (\, \frac{\partial h}{\partial z} - 1\,)\,] - S_w(t, z, h) \tag{94}$$

where the function $C(h) = d\theta/dh$ $[mm^{-1}]$ is called specific soil water capacity and $K(h)$ $[mm\ d^{-1}]$ denotes the unsaturated hydraulic conductivity as a function of the matric potential.

1.4.2 Hydraulic Functions

For the application of the Richards equation (94) in soil water flow simulations the coefficients of the equation have to be known. That means, the following functions of the matric potential h,

a) the water retention $\theta(h)$, i.e. the volumetric water content θ at matric potential h,

b) it's slope, the specific water capacity $C(h) = \dfrac{d\theta}{dh}$ and

c) the unsaturated hydraulic conductivity $K(h)$

have to be given, if possible, in a form, which can be evaluated with relative ease. Hence, to represent the hydraulic functions in a useful way numerous different mathematical closed form expressions have been formulated and applied (Leij et al., 1997). These representations are referred to as 'parametric models' or 'parameterisations' of the hydraulic functions, since they provide a small set of parameters by which the form of the functions is completely determined. The values of these parameters are obtained by fitting the corresponding parametric models to the measured hydraulic functions. Thus, only a few parameter values are sufficient to represent the hydraulic properties needed to simulate soil water flow with Richards equation. Furthermore, using comprehensive datasets on measured soil hydraulic properties pedotransfer functions can be derived, such that parameter values for parameterisations of soil hydraulic functions can be determined by basic soil properties including data on texture, bulk density and organic matter content (van Alphen et al., 2001). Since soil horizons can have considerably different soil hydraulic properties, parameter values are needed for each single soil horizon.

In EXPERT-N the following parametric models according to

- van Genuchten (1980) - Mualem (1976),
- Brooks and Corey (1966) - Burdine (1953),
- Hutson and Cass (1987) - Burdine (1953), and
- Brutsaert (1966) - Gardner (1958)

are provided as the standard parameterisations for the hydraulic functions.

Moreover, in EXPERT-N additional parametric models to represent hydraulic functions can be chosen, in particular for bimodal hydraulic functions. If measurements are available, parameter values can be estimated using the fitting and optimization routines of EXPERT-N. If measured data on hydraulic properties are lacking, but basic soil properties are known, pedotransfer functions are used EXPERT-N to determine the soil hydraulic parameter values which are needed.

1.4.2.1 van Genuchten - Mualem Parameterisation

The today most widely used parametric model is the model of van Genuchten (1980):

$$\theta(h) \;=\; \theta_{res} \;+\; (\theta_{sat} - \theta_{res})\;[\;1 \;+\; (\alpha\;|h|)^n\;]^{-m} \tag{95}$$

$$h(\theta) \;=\; -\,\frac{1}{\alpha}\;\left[\;\left(\frac{\theta - \theta_{res}}{\theta_{sat} - \theta_{res}}\right)^{-1/m} \;-\; 1\;\right]^{1/n} \tag{96}$$

h	matric potential $[mm]$
θ	volumetric water content $[mm^3\;mm^{-3}]$
θ_{sat}	saturated volumetric water content $[mm^3\;mm^{-3}]$
θ_{res}	residual volumetric water content $[mm^3\;mm^{-3}]$
α, n, m	van Genuchten α $[mm^{-1}],\;\alpha > 0$, van Genuchten n [1] and m [1], $n > 0,\;m > 0$, often $m = 1 - 1/n$ is assumed, see equation (99)

$\theta_{sat}, \theta_{res}, \alpha, n, m$ are the parameters which can be determined by matching the parametric model to experimental data. Often the saturated volumetric water content θ_{sat} is set equal to the porosity ϕ and θ_{res} is set to zero. But in field experiments, because of entrapped air and large pores which drain so fast that they get not saturated, θ_{sat} is often found to be smaller than porosity. Moreover, the residual water content θ_{res} which is thought to indicate adsorbed water, is mainly used as a pure shape parameter giving an additional degree of freedom for curve fitting.

The unsaturated hydraulic conductivity is calculated using the general model of Mualem (1976) and Mualem and Dagan (1978), i.e. by the following integral formula:

$$K(S_0) = K_{sat}\;S_0^p\;\left(\frac{\displaystyle\int_0^{S_0} |h(S)|^{-q}\;dS}{\displaystyle\int_0^{1} |h(S)|^{-q}\;dS}\right)^r \tag{97}$$

Here, the relative saturation S_0 [1] at the matric potential h_0 $[mm]$ is defined by:

$$S_0 = S(h_0) = \frac{\theta(h_0) - \theta_{res}}{\theta_{sat} - \theta_{res}} \tag{98}$$

$K(S_0)$	unsaturated hydraulic conductivity K $[mm\;d^{-1}]$ as function of relative saturation S_0 [1]
K_{sat}	saturated hydraulic conductivity $[mm\;d^{-1}]$
h	matric potential $[mm]$
θ	volumetric water content $[mm^3\;mm^{-3}]$
θ_{sat}	saturated volumetric water content $[mm^3\;mm^{-3}]$
θ_{res}	residual volumetric water content $[mm^3\;mm^{-3}]$
p, q, r	parameter values [1], which can be estimated by curve fitting to experimental data: $p > 0,\;q > 0,\;r > 0$; acc. Mualem (1976) $p = \frac{1}{2},\;q = 1$ and $r = 2$.

Using the van Genuchten parameterisation with the restriction $m = 1 - q/n$ results the following expression for the unsaturated hydraulic conductivity $K(h)$ $[mm\ d^{-1}]$ as a function of the matric potential h $[mm]$ (van Genuchten, 1980):

$$K(h) \ = \ K_{sat} \left\{[1 + (\alpha|h|)^n]^{q/n-1}\right\}^p \left\{1 - (\alpha|h|)^{n-q} \ [1 + (\alpha|h|)^n]^{q/n-1}\right\}^r \tag{99}$$

Without the restriction on the parameter m a mathematical expression for $K(h)$ $[mm\ d^{-1}]$ was given by van Genuchten and Nielsen (1985), which is in fact more general but also more difficult to evaluate:

$$K(h) \ = \ K_{sat} \left\{[1 + (\alpha|h|)^n]^{-m}\right\}^p \ [I_x(u,v)]^r \tag{100}$$

$K(h)$	unsaturated hydraulic conductivity $[mm\ d^{-1}]$
h	matric potential $[mm]$
K_{sat}	saturated hydraulic conductivity $[mm\ d^{-1}]$
α, n, m	van Genuchten α $[mm^{-1}],\ n$ [1], m [1]
p, q, r	parameter values [1], acc. Mualem (1976) $p = \frac{1}{2},\ q = 1$ and $r = 2.$
$I_x(u,v)$	incomplete Beta-function, which is calculated by continued fractions, where $x = [1 + (\alpha|h|)^n]^{-m}$, $u = m + q/n$ and $v = 1 - q/n$, $u > 0,\ v > 0$

1.4.2.2 Brooks and Corey - Burdine Parameterisation One of the precursors of the van Genuchten parametric model is the model of Brooks and Corey (1966):

$$\theta(h) \ = \ \begin{cases} \theta_{res} + (\theta_{sat} - \theta_{res}) \ (h/a)^{-\lambda} & \text{for } h < a \\ \quad \theta_{sat} & \text{for } a \leq h \end{cases} \tag{101}$$

$$h(\theta) \ = \ a \left(\frac{\theta - \theta_{res}}{\theta_{sat} - \theta_{res}}\right)^{-1/\lambda} \qquad \text{for } \theta < \theta_{sat}, \tag{102}$$

(for $\theta = \theta_{sat}$, i.e. for $h \geq a$, the function $\theta(h)$ cannot be inverted).

h	matric potential $[mm]$
θ	volumetric water content $[mm^3\ mm^{-3}]$
θ_{sat}	saturated volumetric water content $[mm^3\ mm^{-3}]$
θ_{res}	residual volumetric water content $[mm^3\ mm^{-3}]$
λ	Brooks and Corey exponent [1]
a	air entry value or characteristic length of the soil $[mm]$

Near saturation it is assumed that θ remains constant, $\theta = \theta_{sat}$, until the matric potential falls below the value of a, the air entry value. Then the relative saturation decreases exponentially with further decreasing matric potential. The slope $d\theta/dh$ of the retention function, i.e. the specific water capacity is discontinuous at a. Hence, the Brooks and Corey parameterisation is not smooth (not continuously differentiable) near saturation.

For $\alpha|h| \gg 1$ the parametric model of Brooks and Corey is a good approximation of the van Genuchten model, if we set $a = -\alpha^{-1}$ and $\lambda = mn$. Therefore, the physical interpretation of the parameter van Genuchten α is usually to be the inverse air entry value of the soil.

From the model of Burdine (1953), i.e. from equation (98) with p=2, q=2 and r=1, results the following expression for the unsaturated conductivity $K(h)$ $[mm\ d^{-1}]$:

$$K(h) \; = \; \begin{cases} K_{sat}\ (h/a)^{-2-3\lambda} & \text{for } h < a \\ \quad K_{sat} & \text{for } a \leq h \end{cases} \tag{103}$$

h	matric potential $[mm]$
K_{sat}	saturated hydraulic conductivity $K(h)$ $[mm\ d^{-1}]$
λ	Brooks and Corey exponent [1]
a	air entry value $[mm]$

1.4.2.3 Hutson and Cass - Burdine Parameterisation Following the model LEACHN (Hutson and Wagenet, 1992), the parametric model of Hutson and Cass (1987) can also be used in EXPERT-N:

$$\theta(h) \; = \; \begin{cases} \theta_{sat}\ (h/a)^{-1/b} & \text{for } h_i > h \\ \theta_{sat}\ [\, 1 \; - \; (h/a)^2\ (2b)^{-1}\ (h/a)^{-2-1/b}] & \text{for } 0 \geq h \geq h_i \end{cases} \tag{104}$$

$$h(\theta) = \begin{cases} a\ (\theta/\theta_{sat})^{-b} & \text{for } \theta < \theta_i \\ a\ (1-\theta/\theta_{sat})^{\frac{1}{2}} (\theta_i/\theta_{sat})^{-b} (1-\theta_i/\theta_{sat})^{-\frac{1}{2}} & \text{for } \theta_i \leq \theta \leq \theta_{sat} \end{cases} \tag{105}$$

h	matric potential $[mm]$
θ	volumetric water content $[mm^3\ mm^{-3}]$
θ_{sat}	saturated volumetric water content $[mm^3\ mm^{-3}]$
θ_i/θ_{sat}	$= 2b/(1+2b)$ [1]
h_i	$= a\ [2b/(1+2b)]^{-b}$ $[mm]$
a	air entry value $[mm]$, parameter value to be fitted (Campbell A)
b	parameter value to be fitted (Campbell B) [1], corresponds to the inverse of the Brooks and Corey exponent λ, i.e. $b = \lambda^{-1}$

To obtain a smooth transition zone from the unsaturated to the saturated part of the curve the exponential function is extended to $h_i \leq h \leq 0$ by a parabolic function, in a way that no additional parameters are needed. Furthermore, the derivation $d\theta/dh$ is continuous, thus, also at h_i, which is the inflection point of the curve.
For each soil horizon the empirical constants a and b, so-called Campbell A and B, are estimated by matching the parametric model to the measured retention function. They can also be calculated from basic soil data on texture, bulk density and organic matter, respectively, carbon content of the considered soil horizon by the use of pedotransfer functions. Note that for this parametric model the residual water content is set to zero.

The hydraulic conductivity can be obtained from equation (98) with p=2, q=2 and r=1, i.e. by the model of Burdine (1953):

$$K(h) = K_{sat}\ (h/a)^{-2-3/b} \ \text{ for } h < h_i \tag{106}$$

$$K(\theta) = K_{sat}\ (\theta/\theta_{sat})^{2b+3} \ \text{ for } \theta \geq \theta_i \tag{107}$$

$K(h), K(\theta)$	hydraulic conductivity $[mm\ d^{-1}]$ as a function of θ or h
h	matric potential $[mm]$
θ	volumetric water content $[mm^3\ mm^{-3}]$
K_{sat}	saturated hydraulic conductivity $[mm\ d^{-1}]$
θ_{sat}	saturated volumetric water content $[mm^3\ mm^{-3}]$
a, b	Parameter values of equation (105)

For values of the matric potential of $h < h_i = h(\theta_i)$ the expression for $K(h)$ is applied, else for the corresponding water contents $\theta \geq \theta_i$, the transformed equation for $K(\theta)$ is used.

1.4.2.4 Brutsaert - Gardner Parameterisation The parametric model of Brutsaert (1966) for the retention function is a specific case of the model of van Genuchten (1980) taking $m = 1$. Hence, Brutsaert's model may be seen as a previous specific version of van Genuchten's model. The same function type was used by Gardner (1958) for the parameterisation of the unsaturated conductivity function, see also (Vachaud and Vauclin, 1975)

$$K(h) \ = \ K_{sat}\ \frac{1}{1 + (A|h|)^B} \tag{108}$$

$K(h)$	unsaturated hydraulic conductivity $[mm\ d^{-1}]$ as a function of h
h	matric potential $[mm]$
K_{sat}	saturated hydraulic conductivity $[mm\ d^{-1}]$
A, B	Parameter values Gardner A $[mm^{-1}]$ and Gardner B [1]

In EXPERT-N the Brutsaert-Gardner parameterisation is still used in combination with the pedotransfer function of Vereecken et al. (1989, 1990).

1.4.3 Pedotransfer Functions (PTFs)

The quality of the water flow simulations strongly depends on the accuracy of the soil hydraulic functions that are used. Conventionally the hydraulic functions are derived through laboratory measurements, e.g. by the multistep outflow method (van Dam et al., 1994). Although these measurements can be accomplished in a relatively straight forward way, they are laborious and time-consuming. Therefore, they are also cost-intensive. To reduce these costs alternative methods, so-called pedotransfer functions (Bouma and van Lanen, 1987), have been developed to predict soil hydraulic properties directly from basic soil properties which are more easily determined, such as texture, bulk density and organic matter content (Wösten and van Genuchten, 1988; Vereecken et al., 1989, 1990; Tietje and Tapkenhinrichs, 1993). Two fundamental types of pedotransfer functions can be distinguished: the class pedotransfer functions and continuous transfer functions.

1.4.3.1 Class Pedotransfer Functions For the determination of class pedotransfer functions a comprehensive dataset of measured hydraulic functions for soils of a broad range of different soil types has to be given. Based on such data a class pedotransfer function can be defined, if the soils are grouped into different taxonomic classes with associated average hydraulic functions from the soils belonging to the class. For this purpose the measured hydraulic functions are parameterised e.g. by the van Genuchten parametric model. Hence, the class pedotransfer function assigns to each soil class the corresponding parameter values of the average retention function and the average unsaturated hydraulic conductivity.

Examples are the pedotransfer functions of Clapp and Hornberger (1978), Rawls et al. (1982) and Carsel and Parrish (1988) for the U.S.A., de Jong (1982) for Canada, Wösten et al. (1994) for the Netherlands, Zacharias and Bohne (1997) for Germany.

To obtain the input data needed for the capacity water flow model the EXPERT-N data work bench program uses the class pedotransferfunction of Renger (1971) to calculate retention values at field capacity ($\theta_{fc} = \theta(h_{fc})$, $-3000\ mm \leq h_{fc} \leq -600\ mm$, h_{fc} depending on soil type) and at permanent wilting point ($\theta_{pwp} = \theta(h_{pwp})$, $h_{pwp} = -150000\ mm$).

1.4.3.2 Continuous Pedotransfer Functions Most often datasets from which pedotransfer functions for soil hydraulic functions can be derived also include information on the basic soil properties such as bulk density, texture and organic matter content for each soil horizon. Therefore, often empirical regression equations are obtained, which relate the basic soil properties of a soil horizon to parameters of it’s soil hydraulic functions. In contrast to the average hydraulic function obtained by a class pedotransfer function, for specific basic soil properties also specific hydraulic functions can be determined from regression equations, which consequently are called continuous pedotransfer functions.

In EXPERT-N the choice is between the continuous pedotransfer functions of Campbell (1985), Rawls and Brakensiek (1985) and Vereecken et al. (1989, 1990).

In the following ’$\log$’ denotes the natural logarithm, i.e. the inverse of the exponential function ’$\exp$’.

a) PTF of Campbell Input data for the pedotransfer function of Campbell (1985) are the soil bulk density ρ_s [mg mm^{-3}] and the textural data, i.e. fractions of sand f_{sand} [1], silt f_{silt} [1] and clay f_{clay} [1]. The pedotransfer function itself is finally given by the following regression equations for the parameters a [kPa] (Campbell A) and b [1] (Campbell B), and for the saturated hydraulic conductivity K_{sat} [m s^{-1}] :

$$\begin{aligned} a &= -\,0.5\, d_g^{-1/2}\, (\rho_s/1.3)^{0.67b} && (109)\\ b &= d_g^{-1/2} \,+\, 0.2\, \sigma_g && (110)\\ K_{sat} &= 3.9\; 10^{-5}\, (1.3/\rho_s)^{1.3b}\, \exp(-6.9\, f_{clay} \,-\, 3.7\, f_{silt}) && (111) \end{aligned}$$

where the geometric mean particle diameter d_g [mm] and it’s geometric standard deviation σ_g [1] (Shirazi and Boersma, 1984) are calculated as follows (Campbell, 1985):

$$\begin{aligned} d_g &= \exp(e_g) && (112)\\ e_g &= f_{clay} \log(d_{clay}) + f_{silt} \log(d_{silt}) + f_{sand} \log(d_{sand}) && (113)\\ \sigma_g &= \exp(f_g) && (114)\\ f_g &= [\, f_{clay} \log(d_{clay})^2 + f_{silt} \log(d_{silt})^2 + f_{sand} \log(d_{sand})^2 \,-\, e_g^2\,]^{1/2} && (115) \end{aligned}$$

The arithmetic mean particle diameters for the three texture classes are given by $d_{clay} = 0,001$ mm, $d_{silt} = 0,026$ mm and $d_{sand} = 1,025$ mm. They result from the USDA classification (Shirazi and Boersma, 1984) of particle diameters into texture classes (clay: $0 \leq d < 0.002$ mm, silt: $0,002$ mm $\leq d < 0,05$ mm, sand: $0,05$ mm $\leq d \leq 2,0$ mm for the particle diameter d).

For the PTF it is assumed that the saturated volumetric water content θ_{sat} is set equal to the porosity ϕ. If no measurements for ϕ are available, it is calculated by $\phi = 1 - \dfrac{\rho_s}{2,65}$. Furthermore, the residual water content θ_{res} is set to zero. The parameter values for parametric models of van Genuchten, respectively, of Brooks and Corey are estimated using the approximative relations $a = -\alpha^{-1}$, $b = \lambda^{-1}$, and $\lambda = n - 1$ for $m = 1 - 1/n$.

b) PTF of Rawls and Brakensiek To calculate the parameter values of θ_{sat} $[1]$, θ_{res} $[1]$, λ $[1]$ and a $[cm]$ for the Brooks and Corey retention function according to Rawls and Brakensiek (1985) the following PTF is used, for which again input data on soil porosity ϕ and soil texture are needed :

$$\begin{aligned}
\theta_{sat} &= 0.01 - 0.15\ f_{sand} - 0.22\ f_{clay} + 0.98\ \phi \qquad (116)\\
&\quad +0.99\ f_{clay}^2 + 0.36\ \phi f_{sand} - 1.09\ \phi f_{clay}\\
&\quad -0.96\ \phi f_{clay}^2 - 0.24\ \phi^2 f_{sand} + 1.15\ \phi^2 f_{clay}\\
\theta_{res} &= 0.02 + 0.09\ f_{sand} + 0.51\ f_{clay} + 0.03\ \phi \qquad (117)\\
&\quad -1.54\ f_{clay}^2 - 0.11\ f_{sand}\phi - 1.8\ \phi^2 f_{clay}^2\\
&\quad +3.1\ \phi f_{clay}^2 - 0.24\ \phi^2 f_{clay}\\
\log(\lambda) &= -0.78 + 1.78\ f_{sand} - 1.06\ \phi - 0.53\ f_{sand}^2 \qquad (118)\\
&\quad -27.3\ f_{clay}^2 + 1.1\ \phi^2 - 3.1\ \phi f_{sand}\\
&\quad +79.9\ \phi f_{clay}^2 + 2.66\ \phi^2 f_{sand}^2 - 61.1\ \phi^2 f_{clay}^2\\
&\quad -2.4\ f_{sand}^2 f_{clay} - 0.67\ \phi^2 f_{clay}\\
\log(a) &= -5.34 - 18.5\ f_{clay} + 2.48\ \phi + 21.4\ f_{clay}^2 \qquad (119)\\
&\quad +4.36\ \phi f_{sand} + 61.7\ \phi f_{clay} - 14.4\ \phi^2 f_{sand}^2\\
&\quad +85.5\ \phi^2 f_{clay}^2 + 12.8\ f_{sand}^2 f_{clay} - 89.5\ \phi f_{clay}^2\\
&\quad +7.25\ \phi f_{sand}^2 - 5.4\ f_{sand} f_{clay}^2 - 50.0\ \phi^2 f_{clay}
\end{aligned}$$

The parameter values for the other parametric models result in the same way as for the PTF of Campbell from the approximative relations, e.g. $b = \lambda^{-1}$ for the parameter Campbell B or α = $-a^{-1}$ $[cm^{-1}]$ for van Genuchten α.

c) PTF of Vereecken et al. This pedotransfer function is based on the parametric model of van Genuchten for the retention function with $m = 1$. In this case the van Genuchten parametric model coincides with the earlier model of Brutsaert (1966). Using input data on the bulk density ρ_s, soil texture and organic matter content of the soil, the following parameter values of the Brutsaert parameterisation for the retention function can be calculated using the following regression equations with α in $[cm^{-1}]$:

$$\begin{aligned}
\theta_{sat} &= 0.81 - 0.28\ \rho_s + 0.13\ f_{clay} \qquad (120)\\
\theta_{res} &= 0.015 + 0.5\ f_{clay} + 1.39\ f_{Corg} \qquad (121)\\
\log(\alpha) &= -2.49 + 2.5\ f_{sand} - 35.1\ f_{Corg} - 2.62\rho_s - 2.3\ f_{clay} \qquad (122)\\
\log(n) &= 0.05 - 0.9\ f_{sand} - 1.3\ f_{clay} + 1.5\ f_{sand}^2 \qquad (123)
\end{aligned}$$

Again, approximative relations are applied to estimate the parameters for the other parametric models, which are used in EXPERT-N.

Equation (123) of the pedotransfer function may deliver values of $n \leq 1$ for the parameter van Genuchten n. Hence, the application of Mualem's theory (Mualem, 1976), given by equation (97) with $q = 1$, would lead to a zero relative hydraulic conductivity, since, for $n \leq 1$, the integral evalutes as

$$\int_0^\theta \frac{1}{h(x)^q}\,dx \begin{cases} = +\infty & \text{for } \theta = 1 \\ < +\infty & \text{for } \theta < 1 \end{cases} \tag{124}$$

(see appendix). Therefore, Vereecken et al. (1990) additionally developed regression equations to determine the unsaturated conductivity based on the parametric model of Gardner (1958), see equation (108). The following equations of the pedotransfer function determine values for the parameters saturated hydraulic conductivity K_{sat} (in $[cm\ d^{-1}]$!), Gardner A ($[cm^{-1}]$!) and Gardner B [1]:

$$\begin{aligned} \log(K_{sat}) &= 11.04 -\ 0.96\ \log(f_{clay}) -\ 0.66\ \log(f_{sand}) \\ &\quad -\ 0.46\ \log(f_{Corg}) -\ 8.43\ \rho_s && (125) \\ \log(A) &= -0.7 - 1.9\ f_{sand} - 5.8\ f_{clay} && (126) \\ \log(B) &= 0.07 - 0.19\ \log(f_{clay}) - 0.05\ \log(f_{silt}) && (127) \end{aligned}$$

If a measured value for the saturated hydraulic conductivity is available, the regression equation for the parameter Gardner A can be improved (Vereecken et al., 1990):

$$\log(A) = -2.64 - 1.9\ f_{sand} + 5.0\ f_{clay} + 0.51\ \log(K_{sat}) \tag{128}$$

In the case of measured K_{sat} also the general integral of Mualem, equation (97), with $r = 2$ could be applied. But then, the fixed values $p = 2$ and $q = 1$ would give improper estimates for the unsaturated hydraulic conductivities. Therefore, p and q are also determined by regression equations (Vereecken, 1995):

$$\begin{aligned} p &= -0.43 + 1.73\ \log(n) - 0.24\ \log(K_{sat}) && (129) \\ q &= -0.75 - 0.6\ f_{clay} + 0.07\ \log(K_{sat}) + 1.44\ \theta_{sat} && (130) \end{aligned}$$

that not only require the measured K_{sat} $[cm\ d^{-1}]$ value, but also the validity of the inequality $n > q$ for the parameter n of the van Genuchten parameterisation with $m = 1$, see equation (124).

d) PTF of Scheinost et al. The pedotransfer function of Scheinost et al. (1997) for the water retention function was determined for the 1.5 km^2 connected study area of the FAM-Research Station Scheyern (Schröder et al., 2002). Based on values for soil texture bulk density ρ_s $[mg\ mm^{-3}]$ and organic matter content, similar as for the PTF according to Campbell, parameters for the van Genuchten parameterisation with $m = 1$ and α in $[cm^{-1}]$ are determined using the geometric mean particle diameter d_g [mm], its geometric standard deviation σ_g [1] and the following regression equations:

$$\theta_{sat} = 0.85\,\phi + 0.13\,f_{clay} \tag{131}$$

$$\theta_{res} = 0.52\,f_{clay} + 1.6\,f_{Corg} \tag{132}$$

$$\alpha = 10^{-3}\,(0.25 + 4.3\,d_g) \tag{133}$$

$$n = 0.39 + 2.2\,\sigma_g^{-1} \tag{134}$$

where the porosity ϕ [1] is determined by $\phi = 1 - \frac{\rho_s}{2.65}$, and f_{clay} [1], respectively f_{Corg} [1] denote the fractions of clay and organic matter content (determined as kg per kg total soil including the rock or gravel fraction).

For the calculation of the geometric mean particle diameter d_g $[mm]$ and its geometric standard deviation σ_g [1] the average particle diameter of a texture class is determined according to Shirazi et al. (1988) using the geometric mean of the particle size limits of the texture class instead of the arithmetic mean. In particular, the mean particle diameters d_{clay}, d_{silt}, d_{sand}, d_{rock} for the four texture fractions clay (0,04 μm $\leq d < 0,002$ mm), silt (0,002 mm $\leq d < 0,63$ mm), sand (0,63 mm $\leq d < 2,0$ mm) and rock (2,0 mm $\leq d < 63,0$ mm) result from the lower and upper particle size limits of the texture class s_l and s_u by taking $\sqrt{s_l\ s_u}$. For example, for the texture fraction clay the mean value becomes $d_{clay} = \sqrt{0,00004 \text{ mm} \cdot\ 0,002 \text{ mm}} = \sqrt{8\ \cdot\ 10^{-8}}$ mm $= 0,00028$ mm.

This PTF delivers, similarly to the PTF of Vereecken et al. (1989), for the parameter n values with $n < 1$, such that Mualem's theory for the determination of the unsaturated hydraulic conductivity cannot be applied without restriction. Therefore, in EXPERT-N the PTF of Scheinost et al. (1997) is evaluated in connection with the PTF of Vereecken et al. (1990) to get estimates of the unsaturated hydraulic conductivity.

e) PTF of Wösten et al. Using the database HYPRES, which gathers measured soil hydraulic properties of European soils (Wösten et al., 1998, 1999), the following continuous pedotransfer function was developed (Wösten et al., 1998). But, because of the low R^2 values obtained in the regression analysis, it is indicated that the predictions of hydraulic property functions when using this PTF are fairly inaccurate (Wösten et al., 2001):

$$\begin{aligned}
\theta_{sat} &= 0.86 + 0.17 f_{clay} - 0.3 \rho_s - 0.015 f_{silt}^2 + 0.82 f_{orgM}^2 \\
&\quad + 0.0002 f_{clay}^{-1} + 0.0001 f_{silt}^{-1} + 0.015 \log(f_{silt}) \\
&\quad - 0.73 f_{orgM} f_{clay} - 0.06 \rho_s f_{clay} - 0.12 \rho_s f_{orgM} - 0.017 f_{top} f_{silt}
\end{aligned} \tag{135}$$

$$\begin{aligned}
\log(\alpha) &= -13.97 + 3.14 f_{clay} + 3.51 f_{silt} + 64.6 f_{orgM} + 15.29 \rho_s \\
&\quad - 0.19 f_{top} - 4.67 \rho_s^2 - 7.81 f_{clay}^2 - 68.7 f_{orgM}^2 \\
&\quad + 0.0005 f_{orgM}^{-1} + 0.07 \log(f_{silt}) + 0.15 \log(f_{orgM}) \\
&\quad - 4.55 \rho_s f_{silt} - 48.52 \rho_s f_{orgM} + 0.67 f_{top} f_{clay}
\end{aligned} \tag{136}$$

$$\begin{aligned}
\log(n) &= -26.88 - 2.2 f_{clay} + 0.74 f_{silt} - 19.4 f_{orgM} + 45.5 \rho_s \\
&\quad - 7.24 \rho^2 + 3.66 f_{clay}^2 + 28.85 f_{orgM}^2 \\
&\quad - 12.81 \rho^{-1} - 0.0015 f_{silt}^{-1} - 0.0002 f_{orgM}^{-1} \\
&\quad - 0.29 \log(f_{silt}) - 0.07 \log(f_{orgM}) - 44.6 \log(\rho_s) \\
&\quad - 2.26 \rho_s f_{clay} + 8.96 \rho_s f_{orgM} + 0.72 f_{top} f_{clay}
\end{aligned} \tag{137}$$

$$\begin{aligned}
\log(p*) &= 1.05 + 6.19 f_{clay}^2 - 11.36 f_{orgM}^2 - 0.23 \log(f_{orgM})^2 \\
&\quad - 3.54 \rho_s f_{clay} + 0.28 \rho_s f_{silt} + 4.88 \rho_s f_{orgM}
\end{aligned} \tag{138}$$

$$\begin{aligned}
\log(K_{sat}) &= 4.79 + 3.52 f_{silt} + 0.93 f_{top} - 0.97 \rho^2 - 4.84 f_{clay}^2 - 3.22 f_{silt}^2 \\
&\quad + 0.00001 f_{silt}^{-1} - 0.0008 f_{orgM}^{-1} - 0.64 \log(f_{silt}) \\
&\quad - 1.4 \rho_s f_{clay} - 16.73 \rho_s f_{orgM} + 2.99 f_{top} f_{clay} - 3.31 f_{top} f_{silt}
\end{aligned} \tag{139}$$

where $p*$ is defined by $p* = (p+10)/(10-p)$ and p $[1]$ with constraint $-10 < p < +10$ is the parameter p of the Mualem integral (97). f_{clay}, f_{silt} and f_{orgM} denote the fractions of clay, silt and organic matter (in kg per kg soil), α and n are the parameters of the van Genuchten representation of the retention curve with $m = 1 - 1/n$, K_{sat} $[cm\ d^{-1}]$ denotes the unsaturated hydraulic conductivity. For the top soil we set $f_{top} = 1$, else $f_{top} = 0$.

f) PTF of Teepe et al. By means of 1850 measured retention curves for forest soils Teepe et al. (2003) determined a class as well as a continuous pedotransfer functions to estimate parameter values for the van Genuchten parameterisation of the retention curve with $m = 1 - 1/n$. Both pedotransfer functions serve to better represent water retention of forest soils that are different from arable soils mainly by having an undisturbed top soil.
As before, the following pedotransfer functions were calculated using multiple regression. Depending on data for the bulk soil density ρ_s $[mg\ mm^{-3}]$ and soil texture f_{sand} $[1]$, f_{silt} $[1]$, f_{clay} $[1]$ (weight fractions of fine soil) the derived functions provide estimated values for the saturated volumetric water content θ_{sat} $[1]$, for the van Genuchten parameters α $[cm^{-1}]$ and n $[1]$ and for the volumetric water content at permanent wilting point θ_{pwp} $[1]$:

$$\theta_{sat} = 0.98 - 0.37\rho_s \tag{140}$$

$$\begin{aligned}\log(\alpha) = {} & 55.58 - 4.43\rho_s - 20.0f_{silt}^2 - 47.0f_{clay} - 6.6f_{sand}/\rho_s \\ & -36.83f_{sand}^{1/2} - 3.59f_{sand}/\rho_s - 16.0f_{sand}^2 - 36.92f_{silt}^{1/2} \\ & +8.59\log(f_{sand}) + 7.25\log(f_{silt})\end{aligned} \tag{141}$$

$$\log(n-1) = -2.85 + 2.74f_{sand}^2 + 1.64f_{silt} \tag{142}$$

$$\theta_{pwp} = 0.11 + 0.22f_{clay}^{1/2} - 0.09f_{sand} \tag{143}$$

The residual volumetric water content θ_{res} $[1]$ was not included in the multiple regression analysis, since in most cases the residual water content obtained by the fitting procedure was zero. Instead a multiple regression was calculated for the volumetric water content at permanent wilting point θ_{pwp}. Therefore, θ_{res} is estimated applying the van Genuchten parameterisation of the retention curve and inserting the water content value θ_{pwp} given by equation (143) together with the value of the matric potential $h_{pwp} = -1600$ kPa, which defines the permanent wilting point (Teepe et al., 2003).

1.4.4 Numerical Solution of the Richards Equation (LEACHN)

Following the approach of the LEACHN model, soil water flow is simulated by solving the matric potential based form of the Richards equation using numerical approximations.

$$C(h)\,\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[\, K(h)\,\left(\,\frac{\partial h}{\partial z}\; - \;1\,\right)\,\right] \; - \; S_w(t,z,h) \tag{144}$$

t	time $[d]$
z	depth (positively downward) $[mm]$
$h = h(t,z)$	soil matric potential $[mm]$ (in the model the negative pressure of soil suction $[kPa]$ is transformed to $[mm]$ of water head)
$C(h) = \dfrac{\partial \theta}{\partial h}$	differential water capacity as a function of θ or h $[mm^{-1}]$, respectively
$\theta = \theta(t,z)$	volumetric soil water content $[mm^3\; mm^{-3}]$
$K(h)$	hydraulic conductivity as a function of h $[mm\; d^{-1}]$
$S_w(t,z,h)$	sink term for root water uptake $[mm\; mm^{-1}\; d^{-1}]$

1.4.4.1 Finite Difference Discretisation For the numerical solution, which is based on a finite difference method, the one dimensional domain $[0,\ell]$ representing the soil profile is vertically divided into n equidistant layers. To include the boundary conditions two virtual grid points for the the upper and lower end of the soil profile are added to the n grid points that represent the layers. By applying the Crank-Nicolson scheme the resulting finite differences for the time step $\Delta\, t$ from time t^{j-1} to t^j and for the spatial step Δz from node z_{i-1} to z_i is for $(i = 2, ..., n-1)$ given by (Schwarz, 1986):

$$\begin{aligned} C_i^{j-\frac{1}{2}}\;\frac{h_i^j - h_i^{j-1}}{\Delta t} \quad &= \quad \frac{K_{i+\frac{1}{2}}^{j-1}}{\Delta z}\,\left(\,\frac{h_{i+1}^j + h_{i+1}^{j-1}}{2\Delta z} \; - \; \frac{h_i^j + h_i^{j-1}}{2\Delta z} \; - \; 1\,\right) \; - \\ &\quad - \frac{K_{i-\frac{1}{2}}^{j-1}}{\Delta z}\,\left(\,\frac{h_i^j + h_i^{j-1}}{2\Delta z} \; - \; \frac{h_{i-1}^j + h_{i-1}^{j-1}}{2\Delta z} \; - \; 1\,\right) \; - \; S_{w,i}^{j-1} \end{aligned} \tag{145}$$

where

$$C_i^{j-\frac{1}{2}} = \frac{1}{2}[C(h_i^j) + C(h_i^{j-1})],$$

$$K_{i-\frac{1}{2}}^{j-1} = \frac{1}{2}[K(h_i^{j-1}) + K(h_{i-1}^{j-1})], \qquad K_{i+\frac{1}{2}}^{j-1} = \frac{1}{2}[K(h_{i+1}^{j-1}) + K(h_i^{j-1})]$$

These equations together with the corresponding boundary conditions define a tridiagonal equation system, which is nonlinear due to the nonlinear dependency of the hydraulic functions $C(h)$ and $K(h)$ from the matric potential h. The equation system is solved iteratively by successive substitution (Picard iteration): Starting with the solution for the previous

time step and after substitution of the matric potentials obtained during the previous iteration step, a tridiagonal linear equation system results from which new matric potentials are calculated for the next iteration step using the Gauss elimination (or LU-decomposition) method. After maximally 20 steps the iteration is terminated and, in case of convergence of this numerical procedure, the calculated matric potentials give the solution of the Richards equation for the actual time step (Hutson and Wagenet, 1992; Tillotson et al., 1980).
To avoid numerical errors by calculating the differential water capacity only water content values just under the saturation value are admitted ($\theta \leq 0.9999\ \theta_{sat}$).

1.4.4.2 Initial Condition The solution of the Richards equation requires the specification of the initial distribution of the matric potential throughout the whole solution domain $[0, \ell]$ which represents the soil profile:

$$h(t,z) \ = \ h_0(z) \quad \text{for} \quad t = t_0 \ \text{ and } \ 0 \ \leq z \leq \ell \ \ , \tag{146}$$

where h_0 is a prescribed function of z and t_0 is the time when the simulation starts. Although $h_0(z)$ can be any arbitrary function, often for the initial condition a steady-state or equilibrium condition is assumed.

1.4.4.3 Upper Boundary Condition Depending on the given meteorological conditions, by the upper boundary condition we can consider infiltration into the soil profile with or without ponding surface water, as well as evaporation from the soil surface. Three cases are distinguished:

a) infiltration during ponding surface water,

b) unconfined infiltration or evaporation,

c) limited evaporation at the top soil under dry conditions.

At the soil surface, i.e. for z=0, the upper boundary condition is given in each of the three cases in terms of water flow and matric head using a Dirichlet or a flux boundary condition:

$$q_w(t,0) = \begin{cases} -(K\frac{\partial h}{\partial z} \ - \ K) < N + IR - IC - EV & \text{and } h(t,0) = 0 \\ -(K\frac{\partial h}{\partial z} \ - \ K) = N + IR - IC - EV & \text{and } h_{dry} < h(t,0) < 0 \\ -(K\frac{\partial h}{\partial z} \ - \ K) > N + IR - IC - EV & \text{and } h(t,0) = h_{dry} \end{cases} \tag{147}$$

t	time $[d]$	q_w	vol. water flow $[mm\ d^{-1}]$
h	matric potential $[mm]$	K	hydraulic conductivity $[mm\ d^{-1}]$
EV	actual evaporation rate $[mm\ d^{-1}]$	N	precipitation rate $[mm\ d^{-1}]$
IC	interception rate $[mm\ d^{-1}]$	IR	irrigation rate $[mm\ d^{-1}]$
h_{dry}	minimal value of matric potential $[mm]$ at which evaporation is limited due to dry conditions		

First, it is determined which of the three cases exists at the actual time step, before matric potential and hydraulic conductivity of the top numerical soil layer can be calculated. In **case b)** the prescribed precipitation rate $N\ [mm\ d^{-1}]$ (or throughfall $N - IC\ [mm\ d^{-1}]$ or irrigation $IR\ [mm\ d^{-1}]$) diminished by actual evaporation $EV\ [mm\ d^{-1}]$ is lower than the maximal possible infiltration rate as determined by the actual hydraulic conductivity of the top soil, and the infiltration rate equals the prescribed rate. In this case the upper boundary condition is a flux boundary condition or von Neumann condition (Schwarz, 1986) and the top soil matric potential belonging to the prescribed flux rate is determined by iteration. For each rain or irrigation event the actual duration of infiltration results from the given amount of water and the infiltration rate.

Very intensive precipitation events or very high irrigation can lead to a saturation of the top soil because of too small infiltration rates. In this **case a)** the matric potential of the surface soil h_{top} is set to zero and the upper boundary condition becomes a Dirichlet condition (Schwarz, 1986). The infiltration then is limited and ponding water occurs at the soil surface. The retained amount of water infiltrates during the next time steps until it has completely entered the soil or until the next precipitation event starts.

Likewise a Dirichlet condition is applied for the upper boundary in **case c)**, when the soil dries out during longer periods of evaporation without noteworthy rewetting. Initially the upward water flow equals the prescribed potential rate of soil evaporation (von Neumann condition). But, if the top soil gets drier and drier this leads to a water flow that is more and more limited by a low hydraulic conductivity of the top soil resulting in an actual evaporation below the potential rate. If the soil further dries and the soil surface matric potential falls below the given limit h_{dry}, then the upper boundary condition is changed to the Dirichlet condition $h_{top} = h_{dry}$.

By including the upper virtual knot $i = 0$ the discretisation of the Dirichlet condition follows the same scheme as for $i = 1$ and the other knots $(i = 2, ..., n-1)$, but now with a prescribed value ($h_0^j = 0$ or $h_0^j = h_{dry}$) for the matric potential $h_{i-1}^j = h_0^j$ at time j:

$$\begin{aligned} C_1^{j-\frac{1}{2}}\ \frac{h_1^j - h_1^{j-1}}{\Delta t} \quad = \quad & \frac{K_{1\frac{1}{2}}^{j-1}}{\Delta z}\ (\ \frac{h_2^j + h_2^{j-1}}{2\Delta z} \ - \ \frac{h_1^j + h_1^{j-1}}{2\Delta z} \ - \ 1\ ) \ - \\ & - \frac{K_{\frac{1}{2}}^{j-1}}{\Delta z}\ (\ \frac{h_1^j + h_1^{j-1}}{2\Delta z} \ - \ \frac{h_0^j + h_0^{j-1}}{2\Delta z} \ - \ 1\ ) \end{aligned} \qquad (148)$$

The discretisation of the von Neumann condition results from the same scheme by prescribing the water flow $q_{top}\ [mm\ d^{-1}]$ at the upper boundary:

$$C_1^{j-\frac{1}{2}}\ \frac{h_1^j - h_1^{j-1}}{\Delta t} \quad = \quad \frac{K_{1\frac{1}{2}}^{j-1}}{\Delta z}\ (\ \frac{h_2^j + h_2^{j-1}}{2\Delta z} \ - \ \frac{h_1^j + h_1^{j-1}}{2\Delta z} \ - \ 1\ ) \ - \ \frac{q_{top}}{\Delta z} \qquad (149)$$

In both cases the resulting equation has the two unknowns h_1^j and h_2^j.

1.4.4.4 Lower Boundary Condition Also for the lower boundary condition different situations are considered, namely, if unsaturated or saturated conditions prevail at the lower end of the soil profile:

- unsaturated:
    a) free drainage,
    b) prescribed matric potential at the bottom,
    c) zero flux at the bottom,
    d) lysimeter condition.
- saturated:
    e) prescribed daily groundwater level
    f) prescribed daily drainage flux.

Each of these cases is described similar to the upper boundary condition either by a flux boundary condition (von Neumann condition) or by prescribing a value for the matric potential at the lower boundary (Dirichlet condition). If the matric potential h^j_{n+1} is prescribed at the virtual knot $i = n + 1$, the discretisation of the Dirichlet condition for the knot $i = n$ at time j is obtained as for the other knots following the Crank-Nicolson scheme:

$$
\begin{aligned}
C_n^{j-\frac{1}{2}}\ \frac{h_n^j - h_n^{j-1}}{\Delta t} \quad = \quad & \frac{K^{j-1}_{n+\frac{1}{2}}}{\Delta z}\left(\frac{h^j_{n+1} + h^{j-1}_{n+1}}{2\Delta z} - \frac{h^j_n + h^{j-1}_n}{2\Delta z} - 1\right) - \\
& - \frac{K^{j-1}_{n-\frac{1}{2}}}{\Delta z}\left(\frac{h^j_n + h^{j-1}_n}{2\Delta z} - \frac{h^j_{n-1} + h^{j-1}_{n-1}}{2\Delta z} - 1\right)
\end{aligned}
\tag{150}
$$

For a prescribed flux q_{bot} $[mm\ d^{-1}]$ at the bottom of the soil profile the discretisation of the von Neumann condition results in the following equation:

$$
C_n^{j-\frac{1}{2}}\ \frac{h_n^j - h_n^{j-1}}{\Delta t} \quad = \quad \frac{q_{bot}}{\Delta z} - \frac{K^{j-1}_{n-\frac{1}{2}}}{\Delta z}\left(\frac{h^j_n + h^{j-1}_n}{2\Delta z} - \frac{h^j_{n-1} + h^{j-1}_{n-1}}{2\Delta z} - 1\right) \tag{151}
$$

Similar as for the upper boundary condition, both discretized equations have each two unknowns: h^j_n and h^j_{n-1}.

In **case a)**, if free drainage is to be simulated, the von Neumann condition $q_{bot} = K(h^{j-1}_n)$ has to be imposed, i.e. the hydraulic potential at the bottom of the soil profile is supposed to be nearly constant ($\partial h/\partial z = 0$ at $z = z_n$) and the out-flow is only driven by gravitation.

This assumption is valid for groundwater tables far below the depth of the lower end of the considered soil profile.

Case b) is given by prescribing the value of the matric potential at the bottom of the soil profiles as a function of time, it represents the typical Dirichlet condition, whereas for the case of zero flux at the bottom in **case c)** the lower boundary is given by the typical von Neumann condition $q_{bot} = 0$.

Case d) is the lower boundary condition to describe the out-flow from a lysimeter. This is a particular case, which is given as a combination of either prescribing the matric head or the water flux at the bottom of the lysimeter. Lysimeters often have a drainage system or an outlet at the bottom, such that water can drain only if the bottom layer is saturated or has a lower matric potential than that of the suction drainage system. In this case the matric potential at the outlet boundary is set to zero (Dirichlet condition), and during each time step it is checked whether the flux through the bottom is still directed downward (positive). If this is not anymore the case, the lower boundary condition is changed into a von Neumann condition with zero flux, i.e. $q_{bot} = 0$. This condition will be kept as long as the matric potential is negative or below that of the drainage system (Hutson and Wagenet, 1992).

In **case e)** the daily groundwater tables have to be known, such that the matric potential h_n^j $[mm]$ at the lower boundary (for knot n at time j) can be prescribed by the following von Neumann condition:

$$h_n^j \;=\; z_n - z_g + \frac{\Delta z}{2} \tag{152}$$

where z_n is equal to the depth ℓ $[mm]$ of the soil profile and z_g $[mm]$ denotes the depth of the groundwater table. If this boundary condition is chosen, then it is assumed that the groundwater table is within or only slightly below the considered soil profile.

For **case f)** the daily water flow through the lower boundary of the soil profile has to be given. In this case the daily flux is prescribed by a von Neumann condition for the lower boundary and the model simulates a constant flux through the bottom layer of the soil profile for the whole day.

1.4.4.5 Tridiagonal Equation System and LU-decomposition

By the discretisation of the Richards equations one obtains for each single discrete time step t^j $(1 \leq j \leq m)$ of the simulation time an equation system for the unknowns h_i^j at the discrete spatial steps z_i $(1 \leq i \leq n)$, that represent the numerical layers of the soil profile under consideration.

Using the abbreviations

$$a_i = -\frac{1}{2}\,\frac{K_{i-1/2}^{j-1}}{(\Delta z)^2} \tag{153}$$

$$b_i = \frac{1}{2}\,\frac{K_{i+1/2}^{j-1} + K_{i-1/2}^{j-1}}{(\Delta z)^2} + \frac{C_i^{j-1/2}}{\Delta t} \tag{154}$$

$$c_i = -\frac{1}{2}\,\frac{K_{i+1/2}^{j-1}}{(\Delta z)^2} \tag{155}$$

$$d_i = a_i h_{i-1}^{j-1} - (b_i - \frac{2\,C_i^{j-1/2}}{\Delta t})\,h_i^{j-1} - c_i h_{i+1}^{j-1} - \frac{(K_{i+1/2}^{j-1} - K_{i-1/2}^{j-1})}{\Delta z} - S_{w,i}^{j-1} \tag{156}$$

results for $i = 2, \ldots, n-1$ the following equation system for the unknowns $h_{i-1}^j, h_i^j, h_{i+1}^j$:

$$a_i\,h_{i-1}^j \;+\; b_i\,h_i^j \;+\; c_i\,h_{i+1}^j \;=\; d_i \tag{157}$$

From the boundary conditions corresponding equations for the unknowns h_1^j, h_2^j resp. h_n^j, h_{n+1}^j are obtained:

$$b_1 h_1^j \;+\; c_1 h_2^j \;=\; d_1 \quad , \tag{158}$$

$$a_n h_{n-1}^j \;+\; b_n h_n^j \;=\; d_n \tag{159}$$

Overall, an equation system results that is given (in matrix notation) by $\mathbf{A}\,\mathbf{h}^j = \mathbf{d}$ with tridiagonal matrix $\mathbf{A}$:

$$\begin{pmatrix} b_1 & c_1 & 0 & \cdots & \cdots & 0 \\ a_2 & b_2 & c_2 & \ddots & & \vdots \\ 0 & a_3 & b_3 & c_3 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & \cdots & \cdots & 0 & a_n & b_n \end{pmatrix} \begin{pmatrix} h_1^j \\ h_2^j \\ \\ \vdots \\ \\ h_n^j \end{pmatrix} = \begin{pmatrix} d_1 \\ d_2 \\ \\ \vdots \\ \\ d_n \end{pmatrix} \tag{160}$$

As a tridiagonal matrix, the matrix $\mathbf{A}$ can be decomposed into a tridiagonal lower triangular matrix $\mathbf{L}$ and a normalised bidiagonal upper triangular matrix $\mathbf{U}$: (Remson et al., 1971; Engelen-Müllges and Uhlig, 1996; Schwarz, 1986)

$$\mathbf{A} = \mathbf{L}\,\mathbf{U} = \begin{pmatrix} \alpha_1 & 0 & \cdots & \cdots & 0 \\ a_2 & \alpha_2 & \ddots & & \vdots \\ 0 & a_3 & \alpha_3 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & a_n & \alpha_n \end{pmatrix} \begin{pmatrix} 1 & \beta_1 & 0 & \cdots & 0 \\ 0 & 1 & \beta_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \beta_{n-1} \\ 0 & \cdots & \cdots & 0 & 1 \end{pmatrix} \tag{161}$$

if $\alpha_i \neq 0$ is true for all i. By calculating the product $\mathbf{L}\ \mathbf{U}$ and comparing the corresponding entries with that of matrix $\mathbf{A}$ the following relations for α_i and β_i $(i = 1, \ldots, n)$ result:

$$\begin{aligned} \alpha_1 &= b_1 \\ \beta_i &= c_i/\alpha_i \\ \alpha_i &= b_i - a_i\beta_{i-1} \quad (i = 2, \ldots, n) \end{aligned} \tag{162}$$

The decomposition of the matrix serves to determine the solution of the equation system by transforming $\mathbf{A}\mathbf{h}^j = \mathbf{d}$ into the equivalent system $\mathbf{U}\mathbf{h}^j = \mathbf{g}$. At first, the vector $\mathbf{g}$ is calculated from $\mathbf{d} = \mathbf{L}\mathbf{g}$ (forward elimination):

$$g_1 = d_1/\alpha_1, \tag{163}$$

$$g_i = (d_i - a_i g_{i-1})/\alpha_i \quad (i = 2, \ldots, n) \tag{164}$$

After this, equation $\mathbf{U}\mathbf{h}^j = \mathbf{g}$ is solved (backward elimination):

$$h_n^j = g_n, \tag{165}$$

$$h_i^j = g_i - \beta_i h_{i+1}^j \quad (i = n-1, \ldots, 1) \tag{166}$$

1.4.4.6 Picard Iteration Because generally both the elements of the main diagonal b_i and the elements d_i of the right hand side of equation (160) depend over $C_i^{j-1/2} = \frac{1}{2}\left[C(h_i^j) + C(h_i^{j-1})\right]$ nonlinear on the unknowns h_i^j, the discretised Richards equation represents a nonlinear equation system. Its solution can be approximated by using a fixpoint-iteration, the so-called Picard iteration, if sufficiently small time steps are chosen (Schwarz, 1986). For that purpose the values h_i^{j-1} at time step t^{j-1} are inserted as starting values for the first iteration step $h_i^{j,0} := h_i^{j-1}$ into $\mathbf{A}$ and with these inserted values the then linear tridiagonal equation system

$$\mathbf{A}^{j,0}\mathbf{h}^{j,1} = \mathbf{d} \tag{167}$$

is solved by means of the LU-decomposition. By repeated insertion and solution of each in this way linear equation system

$$\mathbf{A}^{j,k}\mathbf{h}^{j,k+1} = \mathbf{d} \tag{168}$$

a series $(\mathbf{h}^{j,k})_k$ results, that is stopped, if the convergence criterion

$$\frac{C_i^{j-1/2,k}}{(\theta_{sat} - \theta_{res})}\,(h_i^{j,k+1} - h_i^{j,k}) < 10^{-3} \tag{169}$$

is met for all $1 \leq i \leq n$, or if a given maximal value for k, the maximal iteration number, is surpassed. In case of convergence, e.g. for the iteration step $k = l_0$, finally as approximative solution $h_i^j := h_i^{j,l_0}$ is obtained.

If no convergence occurs, the iteration procedure is repeated using the first starting values ($h_i^{j,0} := h_i^{j-1}$) again, but applying a smaller time step, that is calculated by a time step control algorithm. If after repeated reduction of the time step the iteration does not converge, the solution procedure is cancelled and the model sends a corresponding error message.

1.4.5 Another Solution of the Richards Equation (HYDRUS)

Based on the alternative procedures of the model HYDRUS (Simunek et al., 1998) this approach simulates soil water flow by numerically solving the mixed form of the Richards equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[\, K(h)\,\left(\,\frac{\partial h}{\partial z}\; - \;1\,\right)\,\right] \; - \; S_w(t,z,h) \tag{170}$$

$t,\ z$	time t $[d]$ and depth z $[mm]$ (oriented towards the centre of earth)
$h = h(t,z)$	matric potential or matric head $[mm]$ (expressed in mm water head)
$\theta = \theta(t,z)$	volumetric soil water content $[mm^3\ mm^{-3}]$
$K(h)$	hydraulic conductivity as function of h $[mm\ d^{-1}]$
$S_w(t,z,h)$	sink term due to root water uptake $[mm\ mm^{-1}\ d^{-1}]$

1.4.5.1 Finite Element Discretisation an often used alternative method of the finite difference discretisation is the finite element method (Schwarz, 1986), which indeed has its particular advantages only for higher dimensional problems and flow regions of complex geometry. The method of finite elements typically applies only to the spatial part of the partial differential equation, whereas the time derivative is still discretised using finite differences. The basic idea of the finite element method (FEM) originates from the calculus of variations (Courant and Hilbert, 1968), which is applied to find extremal functions of certain functionals. Often the search is for a minimum value of an integral expression, which represents the energy of a system. This so-called energy method leads for the FEM-discretisation to an integral expression defining a system of equations, that finally has to be solved by numerical methods (Schwarz, 1986).

In the model HYDRUS (van Genuchten, 1982; Simunek et al., 1998) the finite element method is applied according to the Galerkin method to discretise the one-dimensional Richards equation. For this purpose the interval $[0, \ell]$, that represents the considered soil volume, is divided into n sub-intervals $[z_i, z_{i+1}]$ $(1 \leq i \leq n)$, representing the finite elements i. For each knot z_i, $(1 \leq i \leq n+1)$ the piecewise linear basis function ϕ_i is introduced, which is equal to 1 at knot z_i and zero for all other knots. By this, every continuous, piecewise linear function $f(z)$ on the interval $[0, \ell]$ can be represented as a superposition of basis functions ϕ_i, where the coefficients of ϕ_i are given by the values $f(z_i)$ of the function f at knot z_i. The piecewise linear approximation $\widetilde{h(t,z)}$ of the unknown $h = h(t,z)$ of the

Richards equation (168) therefore can be expressed by the following function:

$$\widetilde{h(t,z)} = \sum_{i=1}^{n+1} \widetilde{h}_i(t)\ \phi_i(z) \quad , \tag{171}$$

where $\widetilde{h}_i(t) := \widetilde{h(t,z_i)}$ is defined for all $1 \le i \le n+1$.
The energy method from the calculus of variations leads to the following condition of orthogonality for each of the $n+1$ basis functions ϕ_i, i.e. to the requirement that the following integrals vanish on the entire solution domain $\Omega = [0,\ell]$:

$$\int_\Omega \{\frac{\partial\theta}{\partial t} - \frac{\partial}{\partial z}[K(\widetilde{h}\,)(\frac{\partial\widetilde{h}}{\partial z} - 1)] + S_w\}\ \phi_i\ dz = 0 \quad , \quad \text{for all} \quad 1 \le i \le n+1 \ . \tag{172}$$

To evaluate these integral equations first integration by parts is applied leading to:

$$\int_\Omega \frac{\partial\theta}{\partial t}\ \phi_i\ dz = K(\widetilde{h}\,)(\frac{\partial\widetilde{h}}{\partial z} - 1)\ \phi_i\ \Big|_{\partial\Omega} - \int_\Omega \{[K(\widetilde{h}\,)(\frac{\partial\widetilde{h}}{\partial z} - 1)]\ \frac{d\phi_i}{dz}\ - S_w\phi_i\ \}dz\ , \tag{173}$$

for all $1 \le i \le n+1$, where $\partial\Omega$ denotes the boundary of the domain Ω.
This transformation of the integral equations permits to include the flux-type boundary condition (von Neumann condition) in a simple way, since the first term of the right hand side is the water flux across the (upper and lower) boundary, and hence here only the prescribed values given by the flux-type boundary condition have to be inserted. Furthermore, using the integration by parts avoids the otherwise arising second derivative, and it suffices as assumed to use basis functions that are only one-times piecewise differentiable.
The insertion of $\sum_{i=1}^{n+1} \widetilde{h}_i\ \phi_i$, which defines the piecewise linear approximation $\widetilde{h}$ leads to

$$\int_\Omega \frac{\partial\theta}{\partial t}\ \phi_i\ dz + \sum_{j=1}^{n+1}\ \widetilde{h_j} \int_\Omega K\frac{d\phi_i}{dz}\frac{d\phi_j}{dz}\ dz = -q_b\ \phi_i\ \Big|_{\partial\Omega} + \int_\Omega K\frac{d\phi_i}{dz}\ dz - \int_\Omega S_w\phi_i\ dz \tag{174}$$

for all $1 \le i \le n+1$, where q_b denotes the water flux across the boundary.

Since the basis functions ϕ_i are in each case at most on two finite elements different from zero, it is advantageous to accomplish the integration element wise per element $\Omega_e = [z_e, z_{e+1}]$, $1 \le e \le n$:

$$\begin{aligned} \sum_e \int_{\Omega_e} \frac{\partial\theta}{\partial t}\ \phi_i\ dz + \sum_{j=1}^{n+1}\ \widetilde{h_j} \sum_e \int_{\Omega_e} K\frac{d\phi_i}{dz}\frac{d\phi_j}{dz}\ dz \quad &= \\ = \ -q_w\ \phi_i\ \Big|_{\partial\Omega} + \sum_e \int_{\Omega_e} K\frac{d\phi_i}{dz}\ dz - \sum_e \int_{\Omega_e} S_w\phi_i\ dz \qquad &, \end{aligned} \tag{175}$$

where the summation $\sum_e$ needs to be carried out only for those elements Ω_e, that include the knot z_i.

To further evaluate the integrals (175) for the term with time derivative the following approximation, also denoted as 'mass lumping', is taken as definition for all $1 \leq i \leq n+1$ (van Genuchten, 1982):

$$\frac{d\theta_i}{dt} \int_{\Omega} \phi_i \, dz \approx \int_{\Omega} \frac{\partial \theta}{\partial t} \, \phi_i \, dz \tag{176}$$

Additionally it is assumed, that the hydraulic conductivity K and also the sink term S_w are continuous, piecewise linear functions on $\Omega = [0, \ell]$, i.e. can be represented similar to the function $\widetilde{h}$ by basis functions ϕ_i ($1 \leq i \leq n+1$), with $K_i(t) = K(t, z_i)$, and $S_i(t) = S(t, z_i)$ representing the values at the knot i:

$$\begin{aligned} K(t,z) &= \sum_{i=1}^{n+1} K_i(t) \, \phi_i(z) && (177) \\ S_w(t,z) &= \sum_{i=1}^{n+1} S_{w,i}(t) \, \phi_i(z) && (178) \end{aligned}$$

Using these definitions, finally the integrals can be explicitly calculated and, for example for a equidistant decomposition of Ω into the finite elements Ω_e each of equal length Δz, the following equation system (in matrix notation) results:

$$\mathbf{B} \, \frac{d\vartheta}{dt} \; + \; \mathbf{A} \, \mathbf{h} \; = \; \mathbf{d} \tag{179}$$

for the vectors ϑ, **h** and **d** as well as for the matrices **A** and **B**, where (van Genuchten, 1982)

$$\begin{aligned} A_{ij} &= \sum_e \int_{\Omega_e} K \frac{d\phi_i}{dz} \frac{d\phi_j}{dz} \, dz = \sum_{e=i}^{i+1} \int_{\Omega_e} \sum_{k=e-1}^{e} K_k \phi_k \frac{d\phi_i}{dz} \frac{d\phi_j}{dz} \, dz = \\ &= \begin{cases} -(K_{i-1} + K_i)/(2\Delta z), & \text{for } i-1 = j \\ (K_{i-1} + 2K_i + K_{i+1})/(2\Delta z) & \text{for } i = j \\ -(K_i + K_{i+1})/(2\Delta z) & \text{for } i+1 = j \\ \qquad 0 & \text{for } |i-k| > 1 \end{cases} \end{aligned} \tag{180}$$

$$B_{ij} = \sum_e \delta_{ij} \int_{\Omega_e} \phi_i \, dz = \sum_{e=i}^{i+1} \delta_{ij} \, \frac{1}{2} \Delta z_e = \begin{cases} \Delta z & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \tag{181}$$

$$\frac{d\vartheta_i}{dt} \; := \; \frac{d\theta_i}{dt} := (\int_{\Omega} \frac{\partial \theta}{\partial t} \, \phi_i \, dz)/(\int_{\Omega} \phi_i \, dz) \qquad \text{'mass lumping'} \tag{182}$$

$$d_i \quad := \quad q_i - g_i - s_i \tag{183}$$

$$q_i \quad = \quad -q_w\, \phi_i \Big|_0^\ell = \begin{cases} -q_{top} & \text{for } z_i = 0 \\ 0 & \text{for } 0 < z_i < \ell \\ q_{bot} & \text{for } z_i = \ell \end{cases} \tag{184}$$

$$g_i \quad = \quad -\sum_e \int_{\Omega_e} K \frac{d\phi_i}{dz}\, dz = \sum_{e=i}^{i+1} \int_{\Omega_e} \sum_{j=e-1}^{e} K_j \phi_j \frac{d\phi_i}{dz}\, dz = -\frac{1}{2}(K_{i-1} - K_{i+1}) \tag{185}$$

$$\begin{aligned} s_i \quad &= \quad \sum_e \int_{\Omega_e} S_w \phi_i\, dz = \sum_{e=i}^{i+1} \int_{\Omega_e} \sum_{j=e-1}^{e} S_{w,j} \phi_j \phi_i\, dz = \\ &= \quad \frac{\Delta z}{6}(S_{w,i-1} + 4S_{w,i} + S_{w,i+1}) \end{aligned} \tag{186}$$

is valid for all $1 < i < n + 1$.

Together with the equations for the boundary conditions a system of ordinary differential equations with nonlinear time-dependent coefficients results, that defines a dynamical system. The discretisation with respect to time necessary for a numerical solution is obtained by a fully implicit finite difference approach ('backward Euler')

$$\mathbf{B}\, \frac{\vartheta^j - \vartheta^{j-1}}{\Delta t} \; + \; \mathbf{A}^j\, \mathbf{h}^j \; = \; \mathbf{d}^j \tag{187}$$

for the time step $\Delta\, t$ between the times t^{j-1} and t^j. Equation (187) represents the now discretised, mixed form of the Richards equation, which finally has to be solved by numerical procedures.

Remark: The Richards equation degenerates from a parabolic to an elliptic partial differential equation if the change from unsaturated to saturated conditions is described, since in this case the term with time derivative vanishes. To guarantee, that the discretised form of the Richards equation is still valid in this case, it has to be ensured, that also the discretised form of the spatial part of the differential equation vanishes (Hornung and Messing, 1984), i.e. that we have for each $1 \leq i \leq n$:

$$\text{If} \quad \frac{(\vartheta^j - \vartheta^{j-1})_i}{\Delta t} \; = \; 0 \;\; , \quad \text{then also} \quad (\mathbf{A}^j\, \mathbf{h}^j)_i \; - \; (\mathbf{d}^j)_i \; = \; 0 \tag{188}$$

This is only fulfilled by the fully implicit discretisation. Therefore, in the case of a non fully implicit numerical solution procedure as given by the Crank-Nicolson scheme of the model LEACHN, reaching of complete saturation $\theta = \theta_{sat}$ is not admitted.

1.4.5.2 Initial Condition As for the solver of the Richards equation of the model LEACHN, at simulation start the initial vertical distribution of the matric head in the soil profile is needed as input, see eq. (147):

$$h(t,z) \;=\; h_0(z) \quad \text{for} \quad t = t_0 \quad , \tag{189}$$

where h_0 denotes the needed vertical input distribution given as function of z and t_0 is the starting time of the simulation. Usually the vertical distribution of the volumetric water contents in the soil profile will be given as start values and the corresponding matric potentials then are determined by applying the chosen water retention curves.

1.4.5.3 Upper boundary condition Generally in the model HYDRUS for water flow simulations as upper boundary condition both a pure Dirichlet condition:

$$h(t,z) \;=\; h_{top}(t) \;\; \text{at the soil surface} \quad z = 0 \quad , \tag{190}$$

and also a pure von Neumann condition:

$$q_w(t,z) \;=\; -K(\frac{\partial h}{\partial z} - 1) \;=\; q_{top}(t) \;\; \text{at the soil surface} \quad z = 0 \quad , \tag{191}$$

can be used.

Additionally also a system dependent upper boundary can be chosen, which is determined by the prevailing atmospheric interface conditions between soil and air. This boundary condition corresponds to the boundary condition for the water flow model according to LEACHN as given by equation (148).

Case a): If the infiltration capacity of the soil is exhausted after strong precipitation events, water builds up at the soil surface, that can flow as run off or may rest as ponding water only very slowly infiltrating into the soil. In this case the boundary condition can be realized by the following 'surface reservoir condition' (Simunek et al., 1998):

$$q_w(t,z) \;=\; -K(\frac{\partial h}{\partial z} - 1) \;=\; q_{top}(t) \;-\; \frac{\partial h}{\partial t} \;\; \text{at the soil surface} \quad z = 0 \quad , \tag{192}$$

where the height of the surface water layer of the ponding water is equal to the positive matric potential $h = h(0,t)$ $[mm]$ at the soil surface. The height of the surface water layer can increase due to precipitation or can reduce due to evaporation and infiltration, described by the flux $q_{top} = N - EV$ denoting the difference between precipitation N and evaporation EV.

Case b): In case of unlimited infiltration or evaporation a Neumann condition is applied.

Case c): If after strong and long lasting evaporation and possible transpiration the soil desiccates and a lower matric potential limit h_{dry} is reached, then evaporation will be limited namely by prescribing the limit value with a Dirichtlet condition.

1.4.5.4 Lower Boundary Condition Also for the lower boundary condition both a pure Dirichlet condition:

$$h(t,z) \;=\; h_{bot}(t) \quad \text{at lower end of profile} \quad z = \ell \quad , \tag{193}$$

and a pure von Neumann condition:

$$q_w(t,z) \;=\; -K(\frac{\partial h}{\partial z} - 1) \;=\; q_{bot}(t) \quad \text{at lower end of profile} \quad z = \ell \quad , \tag{194}$$

can be applied.

Additionally system dependent conditions can be chosen for the lower boundary:

a) free drainage,

b) lysimeter out-flow and

c) drain discharge as a function of groundwater table.

In **case a)** the condition

$$\frac{\partial h}{\partial z} \;=\; 0 \quad \text{at lower end of profile} \quad z = \ell \tag{195}$$

is prescribed, such that the Neumann condition $q_{bot} \;=\; K$ can be inserted.

In **case b)** the out-flow from a lysimeter or a laboratory soil column is described, where the bottom of the soil profile is at free air. Under these conditions drainage occurs, if the soil column is saturated directly above the bottom (Dirichlet condition). However, if the matric potential at the bottom of the soil profile gets negative and as long as it stays negative, no water leaves through the bottom and a zero flux boundary condition (von Neumann condition) applies.

For **case c)** a special relation between groundwater table and drainage at the bottom of the soil profile can be used:

$$q_{bot}(h) = C_1 \exp(C_2 \, |h - \ell|) \tag{196}$$

where h $[mm]$ denotes the matric potential at the lower boundary $z = \ell$ and C_1, C_2 are given input constants (von Neumann condition).

1.4.5.5 Newton-Picard Iteration The mixed form of the Richards equation and its appropriate discretisation by equation (187) implicitly guarantees a coherent water balance. I.e., the calculated water content change of the soil profile between the time steps t^{j-1} and t^j corresponds just the amount of water that entered or left across the boundary of the soil profile or was exchanged by the sink term. This property is described by the nonlinear equation system (187) and has to be conserved during the iteration procedure for the linearisation and solution of the nonlinear equations. Therefore, during the iteration the state variable θ is substituted by a truncated Taylor expansion along h around the expansion point $h_i^{j,k}$, and a mass conserving linearisation is obtained (Hornung and Messing, 1984; Celia et al., 1990; Vogel et al., 1996):

$$\begin{aligned} \theta_i^{j,k+1} &= \theta_i^{j,k} + \frac{d\theta_i}{dt}^{j,k} (h_i^{j,k+1} - h_i^{j,k}) + O(|h_i^{j,k+1} - h_i^{j,k}|) \\ &\approx \theta_i^{j,k} + C_i^{j,k}\,(h_i^{j,k+1} - h_i^{j,k}) \quad , \end{aligned} \tag{197}$$

where $k+1$ and k denote the actual and preceding iteration steps, and $C_i^{j,k} = (d\theta/dh)(h_i^{j,k})$ the differential water capacity at knot i at iteration step k.

By carrying out the fixpoint iteration according to Picard we obtain an iteration procedure, that represents with respect to the nonlinearity of $\theta(h)$ the Newton iteration, but with respect to the other nonlinear dependencies the Picard iteration. Overall the following system of linear recursion equations results:

$$\mathbf{B}\left[\frac{\vartheta^{j,k} + \mathbf{C}^{j,k}\,(\mathbf{h}^{j,k+1} - \mathbf{h}^{j,k}) - \vartheta^{j-1}}{\Delta t}\right] + \mathbf{A}^j\,\mathbf{h}^{j,k+1} = \mathbf{d}^j \tag{198}$$

where the matrix $\mathbf{C}$ is defined as a diagonal matrix by $C_{i,i} = C_i^{j,k}$.

Rearranging and summarising the terms finally leads to the following equation system

$$\mathbf{E}^{j,k}\,\mathbf{h}^{j,k+1} = \mathbf{f}^{j,k} \tag{199}$$

$$\text{mit}\quad \mathbf{E}^{j,k} := \mathbf{B}\,\mathbf{C}^{j,k}/\Delta t + \mathbf{A}^j \tag{200}$$

$$\text{und}\quad \mathbf{f}^{j,k} := (\mathbf{B}\,\mathbf{C}^{j,k}/\Delta t)\,\mathbf{h}^{j,k} - (\mathbf{B}/\Delta t)\,[\vartheta^{j,k} - \vartheta^{j}] + \mathbf{d}^j \tag{201}$$

The equation system (199) is tri-diagonal, because of the insertion of the matric potential values $h_i^{j,k}$ it is also linear and hence can be directly solved during each iteration step by applying the LU-decomposition.

Explicitly we have for $1 < i < n+1$:

$$
\begin{aligned}
E^{j,k}_{i,i-1} &= -\frac{1}{2\Delta z}\,(K^{j,k}_{i-1} + K^{j,k}_{i}) && (202)\\
E^{j,k}_{i,i} &= \frac{1}{2\Delta z}\,(K^{j,k}_{i-1} + 2K^{j,k}_{i} + K^{j,k}_{i+1}) + \frac{\Delta z}{\Delta t}\,C^{j,k}_{i} && (203)\\
E^{j,k}_{i,i+1} &= -\frac{1}{2\Delta z}\,(K^{j,k}_{i} + K^{j,k}_{i+1}) && (204)\\
f^{j,k}_{i} &= \frac{\Delta z}{\Delta t}\,C^{j,k}_{i}\,h^{j,k}_{i} \;+ \frac{1}{2}\,(K^{j,k}_{i-1} - K^{j,k}_{i+1}) - \frac{\Delta z}{6}\,(S^{j-1}_{i-1} + 4S^{j-1}_{i} + S^{j-1}_{i+1}) && (205)\\
&\quad + \frac{\Delta z}{\Delta t}\,(\theta^{j,k}_{i} - \theta^{j-1}_{i}) \;\;,
\end{aligned}
$$

for $i = 1$:

$$
\begin{aligned}
E^{j,k}_{1,1} &= \frac{1}{2\Delta z}\,(K^{j,k}_{1} + K^{j,k}_{2}) + \frac{\Delta z}{\Delta t}\,C^{j,k}_{1} && (206)\\
E^{j,k}_{1,2} &= -\frac{1}{2\Delta z}\,(K^{j,k}_{1} + K^{j,k}_{2}) && (207)\\
f^{j,k}_{1} &= \frac{\Delta z}{\Delta t}\,C^{j,k}_{1}\,h^{j,k}_{1} \;+ \frac{1}{2}\,(K^{j,k}_{1} + K^{j,k}_{2}) - \frac{\Delta z}{6}\,(2S^{j-1}_{1} + S^{j-1}_{2}) && (208)\\
&\quad + \frac{\Delta z}{\Delta t}\,(\theta^{j,k}_{1} - \theta^{j-1}_{1}) \;- q^{j}_{top} \;\;,
\end{aligned}
$$

and for $i = n+1$:

$$
\begin{aligned}
E^{j,k}_{n+1,n} &= -\frac{1}{2\Delta z}\,(K^{j,k}_{n} + K^{j,k}_{n+1}) && (209)\\
E^{j,k}_{n+1,n+1} &= \frac{1}{2\Delta z}\,(K^{j,k}_{n} + K^{j,k}_{n+1}) + \frac{\Delta z}{\Delta t}\,C^{j,k}_{n+1} && (210)\\
f^{j,k}_{n+1} &= \frac{\Delta z}{\Delta t}\,C^{j,k}_{n+1}\,h^{j,k}_{n+1} \;+ \frac{1}{2}\,(K^{j,k}_{n} + K^{j,k}_{n+1}) - \frac{\Delta z}{6}\,(S^{j-1}_{n} + 2S^{j-1}_{n+1}) && (211)\\
&\quad + \frac{\Delta z}{\Delta t}\,(\theta^{j,k}_{n+1} - \theta^{j-1}_{n+1}) \;+ q^{j}_{bot} \;\;.
\end{aligned}
$$

In the same way as for the Picard iteration we obtain also for the Newton-Picard iteration by repeated insertion and solving of the equations (199) a series $(\mathbf{h}^{j,k})_k$, that is truncated, if the convergence criterion (Huang et al., 1996)

$$|\theta^{j,k+1}_{i} - \theta^{j.k}_{i}| = |(\partial\theta/\partial h)^{j,k+1}_{i}\,(h^{j,k+1} - h^{j,k})| \;\leq 0,0001 \qquad (212)$$

is met for all $1 \leq i \leq n+1$ or if the maximal number of permitted iterations is reached.

1.4.6 Actual Evapotranspiration (limitation of the potential rate)

To estimate the actual evaporation per time step $EV_a^{\Delta t}[mm]$ the potential evaporation rate per time step $EV_p^{\Delta t}/\Delta t$ $[mm\ d^{-1}]$ is compared to the maximal possible water flow q_{max} $[mm\ d^{-1}]$ out of the uppermost soil layer (across the soil surface into the atmosphere). q_{max} is calculated using Darcy's law using the hydraulic conductivity $K_1 = K(h_1)$ $[mm\ d^{-1}]$ of the top soil layer and the gradient between matric potential of the uppermost layer $h_1 = h(\theta_1)$ $[mm]$ at volumetric water content θ_1 $[mm^3\ mm^{-3}]$, and the specific matric potential of air dry soil at the soil surface $h_0 =$ -306600 mm water head, that corresponds to a pressure head of -3000 kPa:

$$q_{max} = -K\ \frac{\partial h}{\partial z}\ |_{z=0} = -K_1\ \frac{h_0 - h_1}{\Delta z} \tag{213}$$

Finally the actual Evaporation $EV_a^{\Delta t}$ $[mm]$ during the time interval Δt $[d]$ results by comparing $q_{max}\ \Delta t$ with the potential evaporation $EV_p^{\Delta t}$ $[mm]$:

$$EV_a^{\Delta t} = \min\{EV_p^{\Delta t}/\Delta t; q_{max}\}\ \Delta t \tag{214}$$

If the actual evaporation $EV_a^{\Delta t}$ $[mm]$ is lower than the potential evaporation $EV_p^{\Delta t}$ $[mm]$, i.e. $q_{max}\ \Delta t < EV_p^{\Delta t}$, then the potential transpiration is increased by the corresponding difference $EV_p^{\Delta t} - EV_a^{\Delta t}$. The actual transpiration is then calculated from the root water uptake in the total soil profile, which is limited by the potential transpiration.

1.5 Capacity Model

1.5.1 Water Flow (CERES)

Following the approach of the CERES models (Jones and Kiniry,1986) to simulate soil water flow a capacity model was integrated into EXPERT-N. Using capacity models the soil profile is supposed to exist of several (i.e. n) soil layers, being considered as hydrostatic reservoirs situated one above the other. Each layer i can store a maximal amount of water S_i^{max} $[mm]$ and can dry out to a minimal amount of water S_i^{min} $[mm]$. The minimal water amount is calculated by

$$S_i^{min} = \theta_{pwp,i}\; d_i \tag{215}$$

where for $1 \leq i \leq n$ the volumetric water content at permanent wilting point $\theta_{pwp,i}$ $[mm^3\; mm^{-3}]$ and the thickness of the layer is d_i $[mm]$. The maximal water holding capacity S_i^{max} $[mm]$ results from

$$S_i^{max} = \theta_{max,i}\; d_i \tag{216}$$

defining $\theta_{max,i}$ $[mm^3\; mm^{-3}]$ for each layer by:

$$\theta_{max,i} = \theta_{fc,i} + f_i(\theta_{sat,i} - \theta_{fc,i}) \tag{217}$$

$\theta_{fc,i}$	Vol. water content of layer i at field capacity $[mm^3\; mm^{-3}]$
$\theta_{sat,i}$	soil porosity of layer i $[mm^3\; mm^{-3}]$
f_i	soil factor of layer i (0.5 for sandy and loamy soils 0.4 for all other soils) [1]

Assuming precipitation PR $[mm\; d^{-1}]$, surface runoff RO $[mm\; d^{-1}]$ and evapotranspiration ET $[mm\; d^{-1}]$ being constant during the time step Δt $[d]$, the water flow Q_0 $[mm\; d^{-1}]$ into the top layer is estimated by

$$Q_0 = PR - RO - ET \tag{218}$$

Initially at time t $[d]$ the i-th layer contains an amount of water S_i^t $[mm]$. The amount of water S_i^* $[mm]$, which would be found in the i-th layer at time $t + \Delta t$ $[d]$ if this layer were closed at its bottom, is recursively computed by

$$S_i^* = S_i^t + Q_{i-1}\Delta t \;\;,\;\; 1 \leq i \leq n, \tag{219}$$

where Q_i $[mm\; d^{-1}]$ the flow to the (i+1)-th layer is given by

$$Q_i = \begin{cases} 0 & \text{for } S_i^* \leq S_i^{max} \\ [(S_i^* - S_i^{max})(\theta_{sat,i} - \theta_{fc,i})/\theta_{sat,i}]/\Delta t & \text{for } S_i^* > S_i^{max} \end{cases} \tag{220}$$

Finally the new amount if water $S_i^{t+\Delta t}$ and the new water content is calculated for each layer i by $\theta^{t+\Delta t} = S_i^{t+\Delta t}/d_i$.

$$S_i^{t+\Delta t} = \begin{cases} S_i^* & \text{for } S_i^* \leq S_i^{max} \\ S_i^* - Q_i\Delta t & \text{for } S_i^* > S_i^{max} \end{cases} \tag{221}$$

The surface runoff is estimated using the SCS curve number method. Here, based on a classification of surface soil and climatic conditions, a relationship between precipitation and runoff is chosen by a classification number.

1.5.2 Actual Daily Evapotranspiration - Ritchie (CERES) Method

Actual soil evaporation is estimated by the method of (Ritchie, 1972), which considers two different stages of soil evaporation. During stage one actual soil evaporation EV_{act}^{day} is equal to potential soil evaporation EV_{pot}^{day} until the top soil gets drier and a certain soil-dependent upper limit of cumulative evaporation EL $[mm]$ is reached. Then soil evaporation enters stage two, in which evaporation steadily declines with time. To determine which stage occurs on a day auxiliary variables V $[mm]$ and W $[mm]$ are calculated as sums of the actual evaporation E_{act}^{day} in stage one or stage two. At the beginning of the simulation at time t_0 $[d]$ start values of the variables V and W are given by:

$$V^{t_0} = \begin{cases} EL & \text{for } \theta_{rel,1}^{t_0} < 0,9 \\ 100,0\,(1,0\; - \;\theta_{rel,1}^{t_0}) & \text{for } \theta_{rel,1}^{t_0} \geq 0,9 \end{cases} \tag{222}$$

$$W^{t_0} = \begin{cases} 25.0\; - \;27.8\,\theta_{rel,1}^{t_0} & \text{for } \theta_{rel,1}^{t_0} < 0.9 \\ 0.0 & \text{for } \theta_{rel,1}^{t_0} \geq 0.9 \end{cases} \tag{223}$$

where the relative volumetric water content $\theta_{rel,1}^{t}$ of the top of the layer at time t $[d]$ is defined by

$$\theta_{rel,1}^{t} = (\theta_1^t - \theta_{pwp,1})/(\theta_{fc,1} - \theta_{pwp,1}) \tag{224}$$

θ_1^t	volumetric water content $[mm^3\; mm^{-3}]$ of the top layer at time t
$\theta_{pwp,1}$	volumetric water content $[mm^3\; mm^{-3}]$ of the top layer at permanent wilting point
$\theta_{fc,1}$	volumetric water content $[mm^3\; mm^{-3}]$ of the top layer at field capacity

For the next day, i.e. using a time step $\Delta t \;=\; 1.0$d and identifying daily evaporated water amounts with daily evaporation rates (by multiplying with the factor 1.0d), the actual soil evaporation $EV_{day}^{act,t+\Delta t}$ $[mm]$ at day $t + \Delta t$ and the variables $V^{t+\Delta t}$ and $W^{t+\Delta t}$ are calculated in the case of zero W^t by:

$$V^{t+\Delta t} = \begin{cases} 0.0 & \text{for } I \geq V^t \\ V^t - I + EV_{day}^{pot,t+\Delta t} & \text{for } I < V^t \end{cases} \tag{225}$$

$$W^{t+\Delta t} = \begin{cases} 0.0 & \text{for } V^{t+\Delta t} \leq EL \\ 0.6\ (V^{t+\Delta t} - EL) & \text{for } V^{t+\Delta t} > EL \end{cases} \tag{226}$$

$$EV_{day}^{act,t+\Delta t} = \begin{cases} 0,0 & \text{for } V^{t+\Delta t} \leq EL \\ 0.6\ (V^{t+\Delta t} - EL) & \text{for } V^{t+\Delta t} > EL \end{cases} \tag{227}$$

and if W^t is greater zero, by

$$V^{t+\Delta t} = \begin{cases} V^t & \text{for } I < W^t \\ EL - I + W^t & \text{for } I \geq W^t \end{cases} \tag{228}$$

$$\tau^{t+\Delta t} = \begin{cases} \tau^t + 1.0d & \text{for } I = 0.0 \\ \tau^t & \text{for } 0.0 < I < W^t \\ 0.0 & \text{for } I \geq W^t \end{cases} \tag{229}$$

$$EV_{day}^{act,t+\Delta t} = \begin{cases} \min(EV_{day}^{pot,t+\Delta t};\ 3.5\ \tau^{t+\Delta t} - W^t) & \text{for } I = 0.0 \\ \min(EV_{day}^{pot,t+\Delta t};\ 3.5\ \tau^{t+\Delta t} - W^t + I;\ 0.8\ I) & \text{for } 0.0 < I < W^t \\ EV_{day}^{pot,t+\Delta t} & \text{for } I \geq W^t \end{cases} \tag{230}$$

$$W^{t+\Delta t} = \begin{cases} W^t + EV_{day}^{act,t+\Delta t} - I & \text{for } I < W^t \\ 0.0 & \text{for } I \geq W^t \end{cases} \tag{231}$$

where τ $[d]$ is the time which passed after stage two was reached, $I = PR - RO$ $[mm]$ is the infiltration calculated as difference between daily precipitation PR $[mm]$ and daily runoff RO $[mm]$, and $EV_{day}^{pot,t+\Delta t}$ $[mm]$ is the daily potential evaporation at day $t + \Delta t$ $[d]$.

1.6 Two-Region Water Flow Models

At present different models are proposed to consider non-equilibrium, spatially non-uniform or preferential water flow in soils (Germann and Beven, 1985; Othmer et al., 1991; Jarvis et al., 1991; Chen and Wagenet, 1992; Wilson et al., 1992; Gerke and van Genuchten, 1993; Durner, 1994). All of these models strongly simplify the mechanisms leading to the observed non-equilibrium flow phenomena. In particular, to improve the description of solute transport in structured soils, in EXPERT-N a very simple approach to simulate immobile water can be applied as well as an approach to consider bi-modal pore-systems by special parameterisations of soil hydraulic functions according to Durner (1994) and Priesack and Durner (2006). These models assume that the porous medium consists of two interacting continua one associated with the inter-aggregate or macropore system, and one comprising micropores or the intra-aggregate pores inside soil aggregates (van Genuchten et al., 1999), see Simunek et al. (2003) for a review including also more complex models.

1.6.1 Immobile Water

Occasionally in water flow studies with lysimeters or in field studies the existence of an important fraction of immobile soil water is observed, that is only slowly exchanged with the mobile, percolating soil water. This exchange is described by the following simple modelling approach (Simunek et al., 2001):

$$\frac{d\theta_{imm}}{dt} = \frac{1}{\tau}\left[\frac{\theta_{mob}}{\theta_{sat,mob}} - \frac{\theta_{imm}-\theta_{res}}{\theta_{sat,imm}-\theta_{res}}\right] - S_{w,imm} \quad , \tag{232}$$

θ_{imm}	immobile volumetric water content of the micro-pore region $[mm^3\ mm^{-3}]$
θ_{mob}	mobile volumetric water content of the macro-pore region $[mm^3\ mm^{-3}]$
$\theta_{sat,imm}$	immobile saturated vol. water content of the micro-pore region $[mm^3\ mm^{-3}]$
$\theta_{sat,mob}$	mobile saturated vol. water content of the macro-pore region $[mm^3\ mm^{-3}]$
θ_{res}	residual volumetric soil water content $[mm^3\ mm^{-3}]$
$S_{w,imm}$	root water uptake of immobile water from the micro-pore region $[mm\ mm^{-1}\ d^{-1}]$
τ	first order retention time $[d]$ for water exchange between immobile water in the micro-pore region and mobile water in the macro-pore region.

that is complemented by the following defining equations for the total volumetric soil water content θ $[mm^3\ mm^{-3}]$, for the saturated volumetric soil water content θ_{sat} $[mm^3\ mm^{-3}]$ and for the root water uptake rates $S_w,\ S_{w,mob},\ S_{w,imm}$ $[mm\ mm^{-1}\ d^{-1}]$:

$$\theta = \theta_{mob} + \theta_{imm} \tag{233}$$

$$\theta_{sat} = \theta_{sat,mob} + \theta_{sat,imm} \tag{234}$$

$$S_w = S_{w,mob} + S_{w,imm} \tag{235}$$

If we apply the Richards equation to model soil water flow

$$\frac{\partial \theta_{mob}}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\,(\,\frac{\partial h}{\partial z}\; - \;1\,)\right] \; - \; S_w \; - \; \frac{d\theta_{imm}}{dt} \quad , \tag{236}$$

we get after inserting equation (232) and transforming the Richards equation the following equation to determine θ_{mob}:

$$\frac{\partial \theta_{mob}}{\partial t} = \frac{\partial}{\partial z}\left[K(h)(\frac{\partial h}{\partial z} - 1)\right] - S_{w,mob} - \frac{1}{\tau}\left[\frac{\theta_{mob}}{\theta_{sat,mob}} \; - \; \frac{\theta_{imm} - \theta_{res}}{\theta_{sat,imm} - \theta_{res}}\right] \tag{237}$$

h	soil matric potential $[mm]$
θ_{mob}	mobile volumetric soil water content $[mm^3\ mm^{-3}]$
θ_{imm}	immobile volumetric soil water content $[mm^3\ mm^{-3}]$
θ_{res}	residual vol. soil water content $[mm^3\ mm^{-3}]$
$K(h)$	hydraulic conductivity as function of h $[mm\ d^{-1}]$
τ	first order retention time $[d]$ for the mobile-immobile water exchange
$S_{w,mob}$	root water uptake rate of mobile water from the macro-pore region $[mm\ mm^{-1}\ d^{-1}]$

In this case the applied soil hydraulic functions are representing the mobile water region. For example for the van Genuchten parameterisation of the retention function results

$$\theta_{mob}(h) \; = \; \theta_{sat,mob}\,[\,1 \; + \; (\alpha\,|h|)^n\,]^{-m} \quad , \tag{238}$$

with mobile saturated volumetric water content $\theta_{sat,mob}$ and a zero residual water content for the mobile pore region, since the given residual soil water content is assumed to be associated with the immobile pore region. The immobile soil water content θ_{imm} $[mm^3\ mm^{-3}]$ finally results from integrating equation (232) with time.

1.6.2 Multi-Modal Hydraulic Functions

To better represent retention data of soils with heterogeneous pore systems Durner (1991), Wilson et al. (1992) and Durner (1992) introduced multi-modal retention functions. In combination with Mualem's model for the prediction of the unsaturated conductivity functions from retention curve representations it is possible to derive representations of conductivity curves, that significantly differ from the conductivity functions obtained for uni-modal representations of the retention curve (Durner, 1994). It was shown, that in this way, i.e. by using bi-modal representations, some of the observed patterns of preferential water flow and non-equilibrium solute transport could be simulated by merely applying Darcy's law and Richards equation (Zurmühl and Durner, 1996).

The multi-modal representation of the retention curve for soils with heterogeneous pore systems according to Durner (1991) results from linear superposition of retention functions of the van Genuchten type, that represent different pore subsystems of the considered soil:

$$S = \frac{\theta - \theta_{res}}{\theta_{sat} - \theta_{res}} = \sum_{i=1}^{k} w_i \, S_i \tag{239}$$

for the subcurves

$$S_i = [1 + (\alpha_i \, h)^{n_i}]^{-m_i} \; , \;\; 1 \le i \le k \; . \tag{240}$$

$S = S(h)$	retention curve of the total soil, expressed by relative saturation S [1]
θ	volumetric soil water content $[mm^3 \; mm^{-3}]$
θ_{res}	residual vol. soil water content $[mm^3 \; mm^{-3}]$
θ_{sat}	saturated vol. soil water content $[mm^3 \; mm^{-3}]$
k	number of different pore subsystems [1]
w_i	weighting factors [1] with constraints $0 < w_i < 1$ and $\sum w_i = 1$
$S_i = S_i(h)$	retention curves of the pore subsystems, expressed by relative saturation S_i [1]
h	soil matric head or soil matric potential $[mm]$
α_i, m_i, n_i	van Genuchten parameters α $[mm^{-1}]$, m [1] and n [1] of the i-th retention subcurve with $\alpha_i > 0$, $m_i > 0$ and $n_i > q$ for the parameter q of Mualem's model with $q > 0$, see equations (97) and (243).

To represent the unsaturated hydraulic conductivity curve Mualem's model (Mualem, 1976), i.e. the integral (97) with parameters $p \ge 0$, $q > 0$ and $r > 0$ is applied. By an appropriate substitution the integral is transformed using the dependence on the matric potential h (Fayer and Simmons, 1995; Priesack and Durner, 2006):

$$\begin{aligned} \int_0^{S_0} h(S)^{-q} dS &= \int_{-\infty}^{h_0} h^{-q} \frac{dS}{dh} dh = \int_{-\infty}^{h_0} h^{-q} (\sum_{i=1}^{k} w_i \frac{dS_i}{dh}) dh \qquad (241) \\ &= \sum_{i=1}^{k} w_i \int_{-\infty}^{h_0} h^{-q} \, \frac{dS_i}{dh} dh = \sum_{i=1}^{k} w_i \int_0^{S_i(h_0)} h^{-q} \, dS_i \quad . \qquad (242) \end{aligned}$$

Hence, with $S_0 = S(h_0)$ and $S_{i,0} = S_i(h_0)$ the following equation to calculate the hydraulic conductivity is obtained, if additionally the constrained $m_i = 1 - q/n_i$ according to van Genuchten (1980) is assumed:

$$K(S_0) = K_{sat} \, (\sum_{i=1}^{k} w_i S_{i,0})^p \left(\frac{\sum_{i=1}^{k} w_i \, \alpha_i^q \, [1 - (1 - S_{i,0}^{1/m_i})^{m_i}]}{\sum_{i=1}^{k} w_i \, \alpha_i^q} \right)^r . \tag{243}$$

By this a closed-form expression also a closed-form representation of the hydraulic conductivity as a function of the matric potential h results:

$$K(h) = K_{sat}\,(\sum_{i=1}^{k} w_i\,[1{+}(\alpha_i\,h)^{n_i}]^{-m_i})^p \left(\frac{\sum\limits_{i=1}^{k} w_i\,\alpha_i^q\,\{1-(\alpha_i\,h)^{n_i-q}\,[1+(\alpha_i\,h)^{n_i}]^{-m_i}\}}{\sum\limits_{i=1}^{k} w_i\,\alpha_i^q} \right)^r . \tag{244}$$

More generally, without the constraint $m_i = 1 - q/n_i$, but by using a much more complex numerical evaluation by continued fraction for the incomplete and complete Beta function, see equation (100), we get:

$$K(S_0) = K_{sat}\,(\sum_{i=1}^{k} w_i S_{i,0})^p \left(\frac{\sum\limits_{i=1}^{k} w_i\,\alpha_i^q\,m_i\,I_{\zeta_i}(u_i,v_i)B(u_i,v_i)}{\sum\limits_{i=1}^{k} w_i\,\alpha_i^q\,m_i B(u_i,v_i)} \right)^r , \tag{245}$$

with $\zeta_i = (S_{i,0})^{1/m_i}$, $u_i = m_i + q/n_i$ and $v_i = 1 - q/n_i$, as well as with the notation for the incomplete and complete Beta function, $I_{\zeta_i}(u_i, v_i)$ and $B(u_i, v_i)$, following van Genuchten et al. (1991), see also Press et al. (1992) for the numerical evaluation.

In the model system EXPERT-N by default only the bi-modal representation ($k = 2$) is applied to simulate water flow in soils with two distinct pore systems assuming Darcy-Buckingham's law and solving Richards equation. This bi-modal representation is also applied in the sense of Zurmühl (1994) and Zurmühl and Durner (1996) to calculate mobile and immobile water contents and to describe non-equilibrium solute transport due to preferential water flow. Assuming θ_{imm} $[mm^3\ mm^{-3}]$ represents the water fraction that is kept in the finest pores of a soil, we see from the unsaturated conductivity function of the total pore region that the hydraulic conductivity at θ_{imm} has a finite positive value. That means, the immobile water content θ_{imm} can be defined assuming that there always exists a constant positive ratio between the conductivities at immobile and total water content. Then θ_{imm} can be calculated depending on the total water content θ by using:

$$K[S(\theta_{imm})] \;=\; \epsilon\,K[S(\theta)] \tag{246}$$

$K = K[S(\theta)]$	hydraulic conductivity $[mm\ d^{-1}]$ as a function of the vol. water content θ
θ	volumetric soil water content $[mm^3\ mm^{-3}]$
θ_{imm}	immobile vol. soil water content $[mm^3\ mm^{-3}]$
ϵ	assumed constant ratio [1] between the conductivity of the immobile pore region and the conductivity of the total pore region, determined by a steady state calibration experiment, e.g. $\epsilon = 0.0005$ (Zurmühl and Durner, 1996).

The mobile water content θ_{mob} $[mm^3\ mm^{-3}]$ finally results from the difference between immobile and total soil water content, see equation (233).

1.6.3 Pedotransfer Functions for Bi-Modal Hydraulic Functions

In the same way as the PTFs of Scheinost et al. (1997), see section 1.4.3.2 and equations (131) - (134), also the following pedotransfer functions for the soils of the research station Scheyern (Schröder et al., 2002) were determined. The PTFs that are given by Scheinost (1995) deliver parameter values for the bi-modal representation of the retention curve according to Durner (1994), whereas by the PTF of Priesack et al. (1999) the parameters are estimated for a bi-modal representation of the retention curve, that is made up of two mono-modal curves of the type defined by Brooks and Corey (1966).

1.6.3.1 PTF of Scheinost for Bi-Modal Hydraulic Functions For this bi-modal parameterisation of the retention curve according to Durner (1994) the underlying mono-modal subcurves are of the Brutsaert type, i.e. with van Genuchten parameters $m_i = 1$:

$$\frac{\theta(h) - \theta_{res}}{\theta_{sat} - \theta_{res}} = \frac{w_1}{1 + (\alpha_1 |h|)^{n_1}} + \frac{w_2}{1 + (\alpha_2 |h|)^{n_2}} \tag{247}$$

It is assumed, that θ_{sat} is determined by the total porosity and θ_{res} is given by the value $\theta_{res} = 0.8\ \theta(-150000\text{mm})$. It is further assumed, that the part of the retention curve that represents the macropore region for the matric potentials between 0 mm and -40 mm, can be described by the parameter values $\alpha_1 = 1$ and $n_1 = 5$. By fixing the boundary between macropore and micropore region, i.e. between structural and textural pore region, at the limit value $\theta_{tex} = \theta(-40\text{ mm})$ we get for the parameter w_2:

$$w_2 = \frac{\theta_{tex} - \theta_{res}}{\theta_{sat} - \theta_{res}} \tag{248}$$

because of the relation $w_1 + w_2 = 1$ then also the parameter w_1 is determined.
Hence, only for the parameters $\theta_{sat},\ \theta_{tex},\ \theta_{res},\ \alpha_2$ and n_2 pedotransfer functions have to be determined to obtain from the basic soil parameters the corresponding parameters for the bi-modal representation of the retention curve (Scheinost, 1995):

$$\theta_{sat} = 1 - 0,38\,\rho_s \tag{249}$$

$$\theta_{tex} = 0,86 - 0,34\,\rho_s + 0,14\,f_{clay} \tag{250}$$

$$\theta_{res} = 0,05 + 0,43\,f_{clay} + 1,6\,f_{Corg} \tag{251}$$

$$\log_{10}(\alpha_2) = -1,05 + 0.68\,\log_{10}(d_g) - 0,023\,\sigma_g - 0,5\,\rho_s \tag{252}$$

$$n_2 = 0,26 - 0,17\,\log_{10}(\alpha_2) - 0,0059\,\sigma_g \tag{253}$$

θ_{sat}	saturated vol. water content [1]	ρ_s	soil bulk density [mg mm^{-3}]
θ_{tex}	limit value of textural pore region [1]	f_{clay}	clay fraction of total soil [kg kg^{-1}]
θ_{res}	residual vol. water content [1]	f_{Corg}	org. carbon fraction [kg kg^{-1}]
α_2	van Genuchten α [mm^{-1}] of textural pore region	d_g	geom. mean particle diameter [mm]
n_2	van Genuchten n [1] of textural pore region	σ_g	standard deviation of d_g [1]

Thereby $\log_{10}(\cdot)$ denotes the decadic logarithm that can be related to the natural logarithm $\log(\cdot)$ by use of $\log_{10}(x) = \log(x)/\log(10)$. The geometric mean particle diameter d_g [mm] and its standard deviation σ_g [1] are calculated following Scheinost et al. (1997) (see section 1.4.3.2 d). Finally Scheinost (1995) also determined a pedotransfer function to estimate the saturated hydraulic conductivity K_{sat} for the soils of the study area belonging to the research station Scheyern:

$$\log_{10}(K_{sat}) \;=\; 3,1 \;+\; 0,6\;\log_{10}(d_g) \tag{254}$$

Similarly to the PTF of Scheinost et al. (1997) for the mono-modal parameterisation of the retention curve, also the PTF for the bi-modal parameterisation attains values of $n_2 < 1$ for the parameter n_2. In such cases Mualem's integral cannot be evaluated for $q = 1$, see equation (97) und Gleichung (124). Yet, for most cases we have $n_2 > \frac{1}{2}$, such that the integral equation can be applied for the Mualem parameter $q = \frac{1}{2}$ and therefore an unsaturated hydraulic conductivity curve may be represented, if also values for the Mualem parameters p and r can be determined.

1.6.3.2 PTF of Priesack et al. for Bi-Modal Hydraulic Functions To circumvent the difficulties in evaluating Mualem's integral for small values of the van Genuchten parameters n, Priesack et al. (1999) determined a PTF that is based on the parameterisation of Brooks and Corey (1966). For this purpose first the following bi-modal parameterisation for retention curves was developed

$$\theta(h) = \begin{cases} \theta_{sat} & \text{for } h_b \le h < 0 \\ \theta_a \left(\dfrac{h}{a_1}\right)^{-\dfrac{1}{b_1}} & \text{for } a_2 \le h \le h_b \\ \theta_x \left(\dfrac{h}{a_2}\right)^{-\dfrac{1}{b_2}} & \text{for } -\infty < h \le a_2 \end{cases} \tag{255}$$

using a continuity condition at the transition point a_2 [mm], where both mono-modal sub-curves are composed to build a bi-modal function, as well as the usual continuity condition at the air entry value h_b [mm]

$$a_2 = a_1 \left(\frac{\theta_x}{\theta_a}\right)^{-b_1} \qquad\qquad h_b = a_1 \left(\frac{\theta_{sat}}{\theta_a}\right)^{-b_1} \tag{256}$$

h	matric potential [mm]	θ	vol. water content [1]
h_b	matric potential at air entry value [mm]	θ_{sat}	saturated vol. water content [1]
a_1	matric potential of -40 mm	θ_a	vol. water content [1] at a_1
a_2	matric potential at curve transition point [mm]	θ_x	vol. water content [1] at a_2

Mualem's integral, equation (97) with Mualem parameter values $p = \frac{1}{2}$, $q = 1$ and $r = 2$, can be directly evaluated using the newly developed bi-modal retention curve parameterisation. As result we get the following representation of the hydraulic conductivity without any further constraints on the parameter values:

$$\frac{K(S_e)}{K_{sat}} = \begin{cases} 1 & \text{for } S_a < S_e \leq 1 \\ S_e^p \, \kappa^{-1} \left[\dfrac{S_x^{b_2+1}}{a_2(b_2+1)} + \dfrac{S_e^{b_1+1} - S_x^{b_1+1}}{a_1(b_1+1)} \right]^2 & \text{for } S_x < S_e \leq S_a \\ S_e^{2b_2+2+p} \, \kappa^{-1} \, [a_2(b_2+1)]^{-2} & \text{for } 0 < S_e \leq S_x \end{cases} \tag{257}$$

where

$$\kappa = \left[\frac{S_x^{b_2+1}}{a_2(b_2+1)} + \frac{1 - S_x^{b_1+1}}{a_1(b_1+1)} \right]^2 \tag{258}$$

and

$$S_e = \theta/\theta_{sat} \ , \ S_i = \theta_i/\theta_{sat} \ \text{ for } \ i = a, x$$

Finally, the following relationships define a PTF for the area of the research station Scheyern (Priesack et al., 1999):

$$\theta_a = 0,9 - 0,025 \ \log_{10}(d_g) - 0,38 \, \rho_s \tag{259}$$

$$\theta_\lambda = 0,04 - 0,036 \, d_g + 0,386 \, f_{clay} + 1,7 \, f_{Corg} \tag{260}$$

$$b_2 = -\frac{\log_{10}(a_3/a_2)}{\log_{10}(\theta_\lambda/\theta_x)} \tag{261}$$

For top soils we found:

$$\theta_x = 0,15 + 7,0 \, f_{Corg} + 1,5 \, f_{clay} - 0,015 \, \sigma_g + 0,21 \, \rho_s + 0,18 \ \log_{10}(d_g) \tag{262}$$

$$b_1^{-1} = 0,005 + 0,44 \, (\theta_a - \theta_x) - 0,2 \, f_{Corg} + 0,01 \, \sigma_g \, d_g \tag{263}$$

and for subsoils:

$$\theta_x = 0,87 - 0,05 \ \log_{10}(d_g) - 0,41 \, \rho_s \tag{264}$$

$$b_1^{-1} = 0,06 + 0,05 \log_{10}(d_g) + 0,52(\theta_a - \theta_x) - 0,002\sigma_g + 0,02\rho_s + 0,001\sqrt{\sigma_g/d_g} \tag{265}$$

log_{10}	decadic logarithm	ρ_s	soil bulk density [mg mm^{-3}]
f_{clay}	clay fraction of the total soil [kg kg^{-1}]	f_{Corg}	organic carbon content [kg kg^{-1}]
d_g	geometric mean particle diameter [mm]	σ_g	standard deviation of d_g [1]
a_3	matric potential of -150000 mm	θ_λ	vol. water content [1] at a_3

1.7 Water Flow at Frost

At beginning of ground frost, liquid soil water starts to freeze up to ice. It is assumed, this happens first in the soil macropores and causes a water movement of the still liquid water from the finer pores into the meso- and macropores (Miller, 1980; Williams and Smith, 1995). This leads to a low matric potential in the freezing soil and therefore generates a water flow from the neighboring regions into the freezing zone (Dirksen and Miller, 1966). Besides these effects, in most water flow models that also consider soil freezing, the impact of ice and ice formation on water flow is expressed by a change of unsaturated hydraulic conductivity and described by applying Richards equation. In EXPERT-N the three actually most often used approaches of Flerchinger and Saxton (1989), of Jansson (1999) and of Hansen et al. (1990) were implemented and, if necessary, slightly modified.

1.7.1 Approach of the Model DAISY

The model DAISY (Hansen et al., 1990) simulates water flow by applying Richards equation also at freezing conditions, as long as there is still air in the soil. For this purpose the soil ice content is calculated by an ice formation rate (see section 2.2.3). Additionally, it is assumed, that similarly to the unfrozen soil also under freezing conditions the matric potential is obtained from the volumetric content of liquid water and, vice versa, the volumetric content of liquid water from the matric potential using the hydraulic water retention curve of the unfrozen soil. In the same way it is assumed, that also the unsaturated hydraulic conductivity can be calculated from the soil matric potential or from the volumetric content of liquid soil water using the hydraulic conductivity curve of the unfrozen soil.

In the case when saturation occurs in the freezing zone, i.e. the matric potential gets zero or positive and the pore space is completely filled with ice and liquid water, then water flow is only described by the gravitational flow (positive downward):

$$q_w = K(\theta_{liq}) = K(\theta_{sat} - \theta_{ice}) \tag{266}$$

q_w	vol. water flux $[mm\ d^{-1}]$	$K = K(\cdot)$	unsat. hydr. conductivity curve $[mm\ d^{-1}]$
θ_{liq}	vol. content of liquid water $[1]$	θ_{ice}	vol. ice content $[1]$
θ_{sat}	saturate vol. water content $[1]$		

In this case the unsaturated hydraulic conductivity K results from the hydraulic conductivity function by inserting the volumetric water content of liquid water θ_{liq} [1], which in the case of saturation is given by $\theta_{liq} = \theta_{sat} - \theta_{ice}$. Water flow below the saturated freezing zone is continued to be simulated by Richards equation, in a way, that at the freezing front the water flux out of the freezing zone is prescribed as upper flux boundary condition. This procedure is applied until the soil is no longer frozen and air has entered the soil.

1.7.2 Approach of the Model SHAW

The simulation of water flow at soil frost is accomplished within the model SHAW (Flerchinger and Saxton, 1989) also by using a numerical solution of the Richards equation. For this purpose, under soil freezing conditions, i.e. at soil temperatures below zero degrees Celsius, the matric potential is only additionally expressed in dependence of soil temperature according to Fuchs et al. (1978):

$$h_T = \psi_m/(\rho_w g) = \frac{L_f\, T}{g\,(T + 273)} - \psi_s/(\rho_w g) \tag{267}$$

h_T	matric potential $[m]$	ψ_m	matric potential (as energy density) $[Pa]$
ρ_w	density of water $[kg\ m^{-3}]$	g	acceleration of gravity (9.81 $m\ s^{-2}$)
T	soil temperature [° C]	ψ_s	osmotic potential $[Pa]$
L_f	latent heat of the phase transition between solid-liquid (latent heat of melting) $[J\ kg^{-1}]$		

The osmotic potential ψ_s of the soil solution is calculated by:

$$\psi_s = -c\, R\, T_K \tag{268}$$

ψ_s	osmotic potential $[Pa]$	c	concentration of solutes $[mol\ m^{-3}]$
R	universal gas constant (8,3143 $J\ mol^{-1}K^{-1}$)	T_K	soil temperature in degrees Kelvin $[K]$

Assuming the hydraulic properties of the unfrozen soil as given by water retention and unsaturated conductivity curves can be also applied for the frozen soil, we get from the temperature dependent matric potential h_T the volumetric content of liquid water:

$$\theta_{liq} = \theta(h_T) = \theta\Big[\frac{L_f\, T}{g\,(T + 273)} + \frac{c\, R\,(T + 273)}{\rho_w\, g}\Big] \tag{269}$$

θ_{liq}	vol. content of liquid water [1]	$\theta(h)$	retention curve as function of potential h
h_T	matric potential $[mm]$ after eq. (267)	T	soil temperature [° C] below zero

and correspondingly the hydraulic conductivity $K = K(\theta_{liq})$ $[mm\ d^{-1}]$, such that finally water flow can be simulated by using Richards equation.

Remark: The approach of Fuchs et al. (1978) was developed by considering the osmotic potential (Cary and Mayland, 1972) and by applying the Clausius-Clapeyron equation for the phase transition fluid-solid. For the three-phase system (water vapor - liquid water - ice) during ice formation in unsaturated soil it is assumed, that the soil hydraulic potential is in equilibrium with water vapor directly above the ice and, that in the soil the pressure difference between ice and air is much smaller than that between liquid water and air, see also Zhao et al. (1997) Appendix A, Spaans and Baker (1996). The equation (269) permits to describe the freezing point depression and the freezing characteristic, i.e. the relation $\theta_{liq}(T)$ between volumetric liquid water content θ_{liq} [1] and soil temperature T [° C] near the freezing point.

1.7.3 Approaches of the Model SOILN

Also by the model SOILN (Jansson, 1999) soil water flow during soil freezing is simulated by application of the Richards equation. For this it is assumed as for the other models, that the hydraulic property functions of the unfrozen soil can also be used for the volumetric content of the liquid soil water in frozen or partly frozen soil. Only to avoid an overestimation of water fluxes into the direction towards the freezing front the unsaturated hydraulic conductivity is reduced in this case (Lundin, 1990). This is achieved e.g. by choosing an appropriate averaging of the conductivity values for the concerned numerical soil profile layers (not realised in EXPERT-N), or by a reduction factor:

$$K_f = 10^{-f_{red}\ \theta_{ice}/\theta}\ K \tag{270}$$

K_f	reduced unsaturated hydraulic conductivity $[mm\ d^{-1}]$ for freezing soil
K	unsaturated hydraulic conductivity $[mm\ d^{-1}]$ in freezing soil $K = K(\theta_{liq})$
f_{red}	reduction parameter, $0 \leq f_{red} \leq 10$, depending on freezing conditions in the soil
θ	(total) volumetric water content [1], i.e. $\theta = \theta_{ice} + \theta_{liq}$
θ_{ice}	volumetric ice content $[1]$
θ_{liq}	volumetric content of liquid water $[1]$

The reduction is applied for a negative gradient of the matric potential ($\partial h/\partial z < 0$), such that an upward water flux is reduced, that is directed towards a freezing front advancing from the soil surface deeper into the soil.

Another approach is given by a two-region model to consider preferential water flow in freezing soils and was additionally implemented into the SOILN model by Stähli et al. (1996). This water flow model distinguishes between a pore-region of slow water fluxes, the low flow or matric region, for which the water flow is modelled as previously described, and a pore-region of fast water fluxes, the high flow or macroporous region. This region is particularly needed to describe water fluxes infiltrating into initially air-filled macropores. For the frozen soil it is assumed, that both regions are separated mainly by the ice along the boundaries of the macropores.

The water flow in the macroporous region is then described based on the unit gradient of gravitation and by the following hydraulic conductivity:

$$K_{hf} = K(\theta) - K(\theta_{lf} + \theta_{ice}) \tag{271}$$

K_{hf}	hydraulic conductivity $[mm\ d^{-1}]$ of the macroporous region
$K = K(\cdot)$	unsaturated conductivity function $[mm\ d^{-1}]$
θ	(total) volumetric water content [1], i.e. $\theta = \theta_{lf} + \theta_{ice} + \theta_{hf}$
θ_{ice}	volumetric ice content $[1]$ of the total soil
θ_{lf}	volumetric content of liquid water $[1]$ in the low flow or matric region
θ_{hf}	volumetric content of liquid water $[1]$ in the high flow or macroporous region

During rain fall or snow melting the model simulates water infiltration from the soil surface into the matric region up to a maximal rate, that is determined by the product of the unsaturated hydraulic conductivity $K(\theta_{lf})$ and the hydraulic gradient following Darcy-Buckingham's law. If the potential infiltration rate is higher, i.e. the rate given by the rate of precipitation rate respectively of snow melting surpasses the maximal infiltration rate, the surplus water enters into the air-filled macropores at a rate that is determined by the hydraulic conductivity $K(\theta_{hf})$. If the potential infiltration is even higher water ponding occurs at the soil surface eventually leading to surface run off.

It can be assumed, that water from melting snow, which infiltrates into the macroporous region has a temperature of about $0\ ^{\circ}$C. Therefore it will partly or completely refreeze during infiltration depending on soil temperature. The latent heat released from freezing causes melting of ice in the finer ice-filled pores, hence in the matric region, such that the total volumetric ice content θ_{ice} remains unchanged, but the matric region water content θ_{lf} increases by the same amount of water that freezes in the macroporous region. This redistribution of water during infiltration is calculated by the following water flux from the macroporous into the matric region:

$$q_{tf} = -\,\alpha_h\,\frac{T}{\rho_w L_f} \tag{272}$$

q_{tf}	redistribution rate $[mm\ d^{-1}]$	α_h	heat exchange parameter $[J\ d^{-1}\ ^{\circ}\mathrm{C}^{-1}\ m^{-2}]$
T	soil temperature [° C]	ρ_w	density of water $[kg\ dm^{-3}]$
L_f	latent heat of phase transition between solid-liquid (latent heat of melting) $[J\ kg^{-1}]$		

2 Soil Heat: Transfer and Temperature

2.1 Introduction

To model heat transfer from the land surface into the ground and to simulate the resulting temperature distribution in the soil, we have to consider the near surface distribution of radiant energy and the resulting transport of heat into the soil. Knowledge of the temperature distribution in the soil is particularly important since soil temperature impacts numerous biological processes, such as plant growth or transformation of soil organic carbon and nitrogen pools. Also many other biotic, chemical and physical processes in the soil depend directly or indirectly on the temperature distribution in the soil. In analogy to the transport of chemicals heat transfer in the soil is also called heat transport. It happens mainly by heat conduction, although the convective transport during occurrence of high water flow (e.g. in the event of heavy rainfall) occasionally can be a significant part of heat transfer in the soil.

In the EXPERT-N model, various modelling approaches are used to describe soil heat transport and the temperature development in the soil. This serves on the one hand to compare soil heat transfer models (i.e. a comparison of the different modelling approaches), on the other hand it helps to find a good description of soil freeze and thaw cycles. In Expert-N a reliable temperature model is particularly needed to adequately model N_2O emission dynamics from soil during freeze-thaw cycles. The implemented approaches of the models DAISY (Hansen et al., 1990), SHAW (Flerchinger and Saxton, 1989) and SOILN (Jansson, 1999) are based on a one-dimensional transport equation that includes both heat conduction and heat convection and can also simulate soil freezing. The approach according to the model LEACHN (Hutson and Wagenet, 1992) is based on a simple heat conduction equation without a convective part and without considering the freezing of soil. Finally, the CERES model approach (Jones and Kiniry, 1986) provides a temperature model , which estimates soil temperature using an empirical relationship between soil surface temperature and near surface air temperature.

Except for the last approach, the temperature models each are based on a one-dimensional transport equation, which needs coefficient functions represented by the soil parameter functions heat capacity and heat conduction . These parameter functions depend to a large extent on the mineral composition of the soil, on soil texture, on soil density and on soil moisture and have to be determined for each soil horizon of the considered soil profile. A physically based model after de Vries (1952, 1963) allows to get good estimates of soil heat capacity and soil heat conductivity for most soils, if the basic soil property data (texture, bulk density, organic matter content) of the soil horizons are known and the dynamics of soil moisture distribution in the soil profile can be described.

2.2 Soil Heat Transfer Models

2.2.1 Equations of Soil Heat Transport

2.2.1.1 Law of Soil Heat Flow The law of the vertical one-dimensional heat flow q_h $[J\ m^{-2}\ d^{-1}]$ in unsaturated soil is determined by two parts, by heat transfer due to heat conduction and on the other hand due to heat convection by water flow. Heat conduction is given by Fourier's law, i.e. by the soil temperature gradient and the heat conductivity K_h $[W\ m^{-1}\ {}^{\circ}C^{-1}]$, which is the proportionality factor of this law. The heat convection is calculated by the volumetric heat content of the soil water $H_w = \rho_w c_w T$ $[J\ m^{-3}]$ and the volumetric soil water flow q_w $[m\ d^{-1}]$:

$$q_h = -K_h\,\frac{\partial T}{\partial z}\; + \; q_w\;(\rho_w c_w T) \tag{273}$$

q_h	volumetric heat flow $[J\ m^{-2}\ d^{-1}]$	T	soil temperature [°C]
K_h	heat conductivity of soil $[J\ m^{-1}\ d^{-1}$ °C$^{-1}]$	z	depth $[m]$
q_w	volumetric water flow $[m\ d^{-1}]$	ρ_w	density of water $[kg\ m^{-3}]$
c_w	specific heat capacity of liquid water $[J\ kg^{-1}$ °C$^{-1}]$		

If also flow of water vapor is considered, the equation for the heat flow q_h $[J\ m^{-2}\ d^{-1}]$ extends to:

$$q_h = -K_h\,\frac{\partial T}{\partial z}\; + \; q_w\;(\rho_w c_w T)\; + \; q_v\;(\rho_v c_v T + L_v \rho_w\;) \tag{274}$$

q_h	vol. heat flow $[J\ m^{-2}\ d^{-1}]$	T	soil temperature [°C]
K_h	heat conductivity of soil $[J\ m^{-1}\ d^{-1}$ °C$^{-1}]$	z	depth $[m]$
q_w	vol. water flow $[m\ d^{-1}]$	ρ_w	density of water $[kg\ m^{-3}]$
c_w	specific heat capacity of water $[J\ kg^{-1}$ °C$^{-1}]$	q_v	vol. vapor flux $[m\ d^{-1}]$

2.2.1.2 Law of Heat Conservation The conservation of heat or of heat energy is expressed by the following equation, the continuity equation of heat flow:

$$\frac{\partial H}{\partial t} = -\frac{\partial q_h}{\partial z} + S_h \tag{275}$$

H	vol. heat content of the soil $[J\ m^{-3}]$	t	time $[s]$
q_h	vol. heat flow $[J\ m^{-2}\ d^{-1}]$	z	depth $[m]$
S_h	heat source or sink $[J\ m^{-3}\ d^{-1}]$		

2.2.1.3 Soil Heat Capacity The change of the volumetric heat content dH $[J\ m^{-3}]$ at soil temperature change dT [°C] gives the volumetric soil heat capacity C_h $[J\ m^{-3}\ °\mathrm{C}^{-1}]$:

$$C_h = dH/dT \tag{276}$$

The soil heat capacity is composed by the heat capacities of the different soil compounds here including also the occurrence of ice:

$$C_h = x_m \rho_m c_m\ +\ x_o \rho_o c_o\ +\ x_w \rho_w\, c_w\ +\ x_i \rho_i\, c_i\ +\ x_a \rho_a c_a \tag{277}$$

C_h	vol. heat capacity of the soil $[J\ m^{-3}\ °\mathrm{C}^{-1}]$	x_j	vol. fraction of j [1]
c_j	spec. heat capacity of j $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$	ρ_j	density of j $[kg\ m^{-3}]$,

where $j = m$ for mineral compounds, $j = o$ for organic compounds, $j = w$ for fluid soil water, $j = i$ for soil ice, $j = a$ for soil air, such that the relation $x_m + x_o + x_w + x_i + x_a = 1$ is valid for the volumetric fractions x_j , see e.g. Campbell (1985), S.32, Tab. 4.1. or Table 4.

The contribution of the heat capacity of soil air is small compared to the contributions from the other compounds and is sometimes neglected or only considered by that of water vapor. Additionally the contributions of mineral and organic compounds can be integrated for most mineral soils, since the volumetric heat capacities of both soil fractions are of similar size. Finally we get for the volumetric heat capacity of the soil C_h $[J\ m^{-3}\ °\mathrm{C}^{-1}]$:

$$C_h = \rho_m c_m (1 - \phi)\ + \rho_w c_w \theta\ + \rho_i c_i \theta_i\ + \rho_a c_a x_a \tag{278}$$

ϕ	soil porosity [1]	θ	vol. content of fluid soil water [1]
θ_i	vol. soil ice content [1]	x_a	vol. soil air content
ρ_m	density of min. compounds $[kg\ m^{-3}]$	c_m	specific heat capacity of min. compounds $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$
ρ_w	density of fluid water $[kg\ m^{-3}]$	c_w	specific heat capacity of fluid water $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$
ρ_i	density of ice $[kg\ m^{-3}]$	c_i	specific heat capacity of ice $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$
ρ_a	density of air $[kg\ m^{-3}]$	c_a	specific heat capacity of air $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$

If freezing and thawing and also condensation and evaporation of soil water is considered, we additionally have to account for the heat involved in the phase changes of water. In this case we have to add the energy needed to evaporate the included amount of water vapor from liquid soil water and to substract the energy needed to melt the included soil ice amount. Hence, if we consider the soil heat content change dH $[J\ m^{-3}]$ at the soil temperature change dT [°C] we now get:

$$\frac{\partial H}{\partial T} = \frac{\partial (C_h T)}{\partial T} - L_f\ \rho_{ice}\ \frac{\partial \theta_{ice}}{\partial T} + L_v\ \rho_w \frac{\partial \theta_v}{\partial T} \tag{279}$$

H	vol. soil heat content $[J\ m^{-3}]$	T	soil temperature [°C]
C_h	vol. soil heat capacity $[J\ m^{-3}\ °\mathrm{C}^{-1}]$	L_f	latent heat of fusion $[J\ kg^{-1}]$
θ_{ice}	vol. ice content [1]	ρ_{ice}	density of ice $[kg\ m^{-3}]$
L_v	latent heat of vaporisation $[J\ kg^{-1}]$	θ_v	vol. vapor content [1]
ρ_w	density of fluid water $[kg\ m^{-3}]$		

2.2.1.4 Equation of Heat Transport By applying the law of heat conservation (274), and the law of heat flow (273), we have

$$\begin{aligned}
\frac{\partial H}{\partial t} &= \frac{\partial (C_h T)}{\partial t} - L_f \rho_i \frac{\partial \theta_i}{\partial t} + L_v \rho_w \frac{\partial \theta_v}{\partial t} = -\frac{\partial q_h}{\partial z} + S_h = \\
&= -\frac{\partial}{\partial z}[-K_h \frac{\partial T}{\partial z} + q_w\,(\rho_w c_w T) + q_v\,(\rho_v c_v T + L_v \rho_w\,)] + S_h = \\
&= -\frac{\partial}{\partial z}[-K_h \frac{\partial T}{\partial z}] - \rho_w c_w \frac{\partial (q_w T)}{\partial z} - \rho_v c_v \frac{\partial (q_v T)}{\partial z} - L_v \rho_w \frac{\partial q_v}{\partial z} + S_h
\end{aligned} \tag{280}$$

From which we get the **general soil heat transport equation**, which includes fusion of ice and vaporization of water:

$$\begin{aligned}
&\frac{\partial (C_h T)}{\partial t} - L_f \rho_i \frac{\partial \theta_i}{\partial t} + L_v \rho_w \Big(\frac{\partial \theta_v}{\partial t} + \frac{\partial q_v}{\partial z} \Big) = \\
&= \frac{\partial}{\partial z}\Big[K_h \frac{\partial T}{\partial z} \Big] - \rho_w c_w \frac{(\partial q_w\, T)}{\partial z} - \rho_v c_v \frac{(\partial q_v\, T)}{\partial z} + S_h
\end{aligned} \tag{281}$$

C_h	vol. heat capacity of the soil $[J\ m^{-3}\ °\mathrm{C}^{-1}]$	T	soil temperature [°C]
θ_i	vol. ice content of the soil [1]	ρ_i	density of ice $[kg\ m^{-3}]$
L_f	latent heat of melting $[J\ kg^{-1}]$	L_v	latent heat of vaporization $[J\ kg^{-1}]$
q_w	(non-isothermal) vol. water flow $[m\ s^{-1}]$	q_v	(non-isothermal) vol. vapor flux $[m\ s^{-1}]$
ρ_w	density of water $[kg\ m^{-3}]$	θ_v	vol. vapor content of the soil [1]
K_h	heat conductivity of the soil $[J\ m^{-1} s^{-1}\ °\mathrm{C}^{-1}]$	ρ_v	density of vapor $[kg\ m^{-3}]$
c_w	specific heat capacity of water $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$	c_v	specific heat capacity of vapor $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$

If we now evaluate the first term of the left hand side:

$$\frac{\partial C_h T}{\partial t} = \frac{\partial C_h}{\partial t} T + C_h \frac{\partial T}{\partial t} \tag{282}$$

Under the assumption, that the solid phase of soil, the soil matric is rigid and its volume fraction is not changing we derive:

$$\begin{aligned}
\frac{\partial C_h}{\partial t} &= \frac{\partial}{\partial t}(\rho_m c_m (1-\phi) + \rho_w c_w \theta + \rho_i c_i \theta_i + \rho_v c_v \theta_v) \\
&= 0 + \rho_w c_w \frac{\partial \theta}{\partial t} + \rho_i c_i \frac{\partial \theta_i}{\partial t} + \rho_v c_v \frac{\partial \theta_v}{\partial t}
\end{aligned} \tag{283}$$

Then, by insertion into the general heat transport equation and neglecting the third term of the right hand side of the last equation, since $\rho_i c_i T$ is very small compared to $L_f \rho_i$, i.e. $\rho_i c_i T \ll L_f \rho_i$, and by further differentiation of the right hand side of the transport equation:

$$\begin{aligned}
&C_h \frac{\partial T}{\partial t} + \rho_w c_w \frac{\partial \theta}{\partial t} T + \rho_v c_v \frac{\partial \theta_v}{\partial t} T - L_f \rho_i \frac{\partial \theta_i}{\partial t} + L_v \rho_w \Big(\frac{\partial \theta_v}{\partial t} + \frac{\partial q_v}{\partial z} \Big) = \\
&= \frac{\partial}{\partial z}\Big[K_h \frac{\partial T}{\partial z} \Big] - \rho_w c_w \frac{\partial q_w}{\partial z} T - \rho_w c_w q_w \frac{\partial T}{\partial z} - \rho_v c_v \frac{\partial q_v}{\partial z} T - \rho_v c_v q_v \frac{\partial T}{\partial z} + S_h
\end{aligned} \tag{284}$$

We obtain by inserting into the l.h.s. of (282) **a)** the continuity equation of water flow (Nassar and Horton, 1992; Hansson et al., 2004) for which the vol. ice content θ_i is expressed as equivalent of the vol. water content:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q_w}{\partial z} - \frac{\partial \theta_i}{\partial t} - E + S_w \tag{285}$$

and **b)** the continuity equation of vapor flow (Nassar and Horton, 1992; Sakai et al., 2009)

$$\frac{\partial \theta_v}{\partial t} = -\frac{\partial q_v}{\partial z} + E \tag{286}$$

(expressed as equivalent liquid water flux):

$$\begin{aligned} & C_h \frac{\partial T}{\partial t} + \rho_w c_w \frac{\partial \theta}{\partial t}\, T + \rho_v c_v \frac{\partial \theta_v}{\partial t}\, T - L_f \rho_i \frac{\partial \theta_i}{\partial t} + L_v \rho_w \Big(\frac{\partial \theta_v}{\partial t} + \frac{\partial q_v}{\partial z} \Big) = \\ & = C_h \frac{\partial T}{\partial t} + \rho_w c_w (\frac{-\partial q_w}{\partial z} - \frac{\partial \theta_i}{\partial t} - E + S_w)\, T + \rho_v c_v (\frac{-\partial q_v}{\partial z} + E)\, T - \\ & \quad -L_f \rho_i \frac{\partial \theta_i}{\partial t} \; + L_v \rho_w \Big(E \Big) = \\ & = C_h \frac{\partial T}{\partial t} - \rho_w c_w \frac{\partial q_w}{\partial z}\, T - \rho_w c_w \frac{\partial \theta_i}{\partial t}\, T - \rho_w c_w E\, T + \rho_w c_w S_w\, T - \rho_v c_v \frac{\partial q_v}{\partial z}\, T \\ & \quad + \rho_v c_v E\, T - L_f \rho_i \frac{\partial \theta_i}{\partial t} + L_v \rho_w \Big(E \Big) \end{aligned} \tag{287}$$

where we can neglect the term $\rho_w c_w \frac{\partial \theta_i}{\partial t} T$ because $\rho_w c_w T \ll L_f \rho_w$ and the terms $\rho_w c_w E\; T$ and $\rho_v c_v E\; T$ because $\rho_w c_w T \ll L_v \rho_v$ and $\rho_v c_v T \ll L_v \rho_v$ and re-substitute E in $L_v \rho_w E$ by use of (286) to get:

$$\begin{aligned} & C_h \frac{\partial T}{\partial t} - \rho_w c_w \frac{\partial q_w}{\partial z}\, T + \rho_w c_w S_w\, T - \rho_v c_v \frac{\partial q_v}{\partial z}\, T - L_f \rho_i \frac{\partial \theta_i}{\partial t} + L_v \rho_w \Big(\frac{\partial \theta_v}{\partial t} + \frac{\partial q_v}{\partial z} \Big) \\ & = \frac{\partial}{\partial z} \Big[K_h\, \frac{\partial T}{\partial z} \Big] - \rho_w c_w \frac{\partial q_w}{\partial z}\, T - \rho_w c_w q_w \frac{\partial T}{\partial z} \; - \rho_v c_v \frac{\partial q_v}{\partial z}\, T - \rho_v c_v q_v \frac{\partial T}{\partial z} \; + S_h \end{aligned} \tag{288}$$

Assuming the sink term of heat represents mainly heat lost from the soil volume due to the water sink by root water uptake, we have $S_h = \rho_w c_w S_w\; T$. Then by eliminating terms which occur at either side of the equation (i.e. $-\rho_w c_w \frac{\partial q_w}{\partial z}\; T$, $-\rho_v c_v \frac{\partial q_v}{\partial z}\; T$ and S_h resp. $\rho_w c_w S_w\; T$), we finally have derived a simpler version of the transport equation:

The simplified **soil heat transport equation**, which still considers freezing and melting as well as evaporation and condensation:

$$C_h \frac{\partial T}{\partial t} - L_f \rho_i \frac{\partial \theta_i}{\partial t} + L_v \rho_w \Big(\frac{\partial \theta_v}{\partial t} + \frac{\partial q_v}{\partial z} \Big) = \frac{\partial}{\partial z} \Big[K_h \, \frac{\partial T}{\partial z} \Big] - \rho_w c_w q_w \frac{\partial T}{\partial z} - \rho_v c_v q_v \frac{\partial T}{\partial z} \quad (289)$$

C_h	vol. heat capacity of the soil $[J\ m^{-3}\ °\mathrm{C}^{-1}]$	T	soil temperature [°C]
θ_i	vol. ice content of the soil $[1]$	ρ_i	density of ice (=916.7 $kg\ m^{-3}$)
L_f	latent heat of melting $[J\ kg^{-1}]$ $(= 3.34\ 10^5 J\ kg^{-1})$	L_v	latent heat of vaporization $[J\ kg^{-1}]$ $(= 2.501\ 10^6 - 2.3692T\ J\ kg^{-1})$
q_w	(non-isothermal) vol. water flow $[m\ s^{-1}]$	q_v	(non-isothermal) vol. vapor flow $[m\ s^{-1}]$
ρ_w	density of water $(= 1.0\ 10^3\ kg\ m^{-3})$	θ_v	vol. vapor content of the soil $[1]$
K_h	heat conductivity of the soil $[J\ m^{-1} s^{-1}\ °\mathrm{C}^{-1}]$	ρ_v	density of vapor $(= 958.0\ kg\ m^{-3})$
c_w	specific heat capacity of water (= 4.186 $kJ\ kg^{-1}\ °\mathrm{C}^{-1}$)	c_v	specific heat capacity of vapor (= 2.108 $kJ\ kg^{-1}\ °\mathrm{C}^{-1}$)

2.2.1.5 Non-isothermal Liquid Water and Water Vapor Flow In the non-isothermal case the liquid water flux q_w is described by a modified Darcy-Buckingham law (Philip and de Vries, 1957) by including the non-isothermal liquid water flow $q_{wT} = -K_{wT} \, \frac{\partial T}{\partial z}$:

$$q_w = q_{w\psi} + q_{wT} = -K_{w\psi} \, \frac{\partial \psi}{\partial z} + K_{w\psi} \, - K_{wT} \, \frac{\partial T}{\partial z} \quad (290)$$

Similar the vapor flux q_v (expressed as an equivalent liquid water flux) is separated into an isothermal flux $q_{v\psi}$ and an non-isothermal flux q_{vT}:

$$q_v = q_{v\psi} + q_{vT} = -K_{v\psi} \, \frac{\partial \psi}{\partial z} - K_{vT} \, \frac{\partial T}{\partial z} \quad (291)$$

Then expressing θ_i and θ_v in equivalent water contents, we obtain for the total water content $\theta_g = \theta + \theta_i + \theta_v$ by combining liquid and vapor water fluxes a general equation of non-isothermal water flow (Saito et al., 2006; Sakai et al., 2009; Vanderborght et al., 2017):

$$\frac{\partial \theta_g}{\partial t} = \frac{\partial}{\partial z} \Big[K_{w\psi} \frac{\partial \psi}{\partial z} - K_{w\psi} + K_{wT} \frac{\partial T}{\partial z} + K_{v\psi} \frac{\partial \psi}{\partial z} + K_{vT} \frac{\partial T}{\partial z} \Big] \, - S \quad (292)$$

θ_g	total vol. soil water content $[cm^3\ cm^{-3}]$	ψ	soil matric potential $[mm]$
T	soil temperature [°C]	S	sink term of liquid water and vapor $[s^{-1}]$
$K_{w\psi}$	isothermal hydraulic conductivity $[m\ s^{-1}]$	K_{wT}	thermal hydraulic conductivity $[m^2\ °C^{-1}\ s^{-1}]$
$K_{v\psi}$	isothermal vapor conductivity $[m\ s^{-1}]$	K_{vT}	thermal vapor conductivity $[m^2\ °C^{-1}\ s^{-1}]$
θ_v	vol. soil vapor content $[cm^3\ cm^{-3}]$	θ_i	vol. soil ice content $[cm^3\ cm^{-3}]$

2.2.1.6 Heat Transport in Frozen Soil For a relatively moist, unsaturated soil the Clausius-Clapeyron equation

$$\frac{dP}{dT} = \frac{L_f}{\rho_w^{-1}\, T} \tag{293}$$

describes the relation between the the tension of liquid soil water $dP = \rho_w\; g\; d\psi$ and the corresponding freezing point depression dT, when the liquid soil water is transformed to ice. Hereby a constant ice gauge pressure and a zero osmotic potential is assumed, cf. Edlefsen and Anderson (1943), p.120, equ. (205). By applying this Clausius-Clayperon equation and inserting $dP = \rho_w\; g\; d\psi$ into (293) we get

$$\frac{d\psi}{dT} = (\rho_w\; g)^{-1} \frac{L_f}{\rho_w^{-1}\, T} = \frac{L_f}{g\, T} \tag{294}$$

and we have for a freezing soil:

$$\begin{aligned} -L_f\; \rho_i\; \frac{\partial \theta_i}{\partial t} &= L_f\; \rho_w\; \frac{\partial \theta}{\partial t} = L_f\; \rho_w\; \frac{\partial \theta}{\partial \psi} \frac{\partial \psi}{\partial T} \frac{\partial T}{\partial t} = L_f\; \rho_w\; \frac{\partial \theta}{\partial \psi} \left(\frac{L_f}{gT} \right) \frac{\partial T}{\partial t} = \\ &= \rho_w\; \frac{L_f^2}{gT} \frac{\partial \theta}{\partial \psi} \frac{\partial T}{\partial t} = \rho_w\; \frac{L_f^2}{gT}\; C(\psi) \frac{\partial T}{\partial t} \end{aligned} \tag{295}$$

and with that, we get from the simplified heat transport equation (289) the modified heat transport equation for freezing soils:

$$\left[C_h + \rho_w \frac{L_f^2}{gT}\; C(\psi) \right] \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} (K_h\; \frac{\partial T}{\partial z}) - \rho_w c_w q_w \frac{\partial T}{\partial z} \; - \rho_v c_v q_v \frac{\partial T}{\partial z} \tag{296}$$

C_h	vol. heat capacity of the soil $[J\; m^{-3}\; °\mathrm{C}^{-1}]$	T	soil temperature [°C]
$C(\psi)$	differential water capacity $[mm^{-1}]$	ψ	matric potential $[mm]$
L_f	latent heat of melting $[J\; kg^{-1}]$	g	acceleration of gravity $[m\; s^{-2}]$
q_w	(non-isothermal) vol. water flow $[m\; s^{-1}]$	q_v	(non-isothermal) vol. vapor flow $[m\; s^{-1}]$
ρ_w	density of water $[kg\; m^{-3}]$	ρ_v	density of vapor $[kg\; m^{-3}]$
K_h	heat conductivity of the soil $[J\; m^{-1}\; s^{-1}\; °\mathrm{C}^{-1}]$		
c_w	specific heat capacity of water $[J\; kg^{-1}\; °\mathrm{C}^{-1}]$	c_v	specific heat capacity of vapor $[J\; kg^{-1}\; °\mathrm{C}^{-1}]$

The term within the square brackets is often called apparent volumetric heat capacity C_a of the soil $[J\; m^{-3}\; °\mathrm{C}^{-1}]$, see (Fuchs et al., 1978; Williams and Smith, 1989; Hansson et al., 2004; Kelleners, 2013).

2.2.2 Thermal Conductivity according to de Vries

The thermal conductivity of the soil strongly depends on the soil composition, i.e. on the volumetric fractions of the different soil compounds. Due to the strong differences between the heat conductivities of water and air the soil heat conductivity depends to a high degree on the water content of the soil. In dry soil heat mainly through the mineral soil particles, but has to bridge air filled gaps between the particles. When water is present it starts to fill these gaps and thus considerably increases the thermal conductivity of the soil due to the higher thermal conductivity of water compared to the thermal conductivity of air. For the description of this complicated situation de Vries (1952, 1963) developed a physically based model of the thermal conductivity of soil. The model is based in analogy to the physical expression for the electrical conductivity or the dielectric constant of a granular material as a function of the volume fractions and the physical properties of its constituents. The basic ideas will be shortly outlined following Hansen et al. (1990).

2.2.2.1 Thermal Conductivity of a Mixture of Granulate Materials It is assumed, that a volume V consists of a continuous medium (e.g. air or water) in which n different types of granulate materials are embedded. The continuous medium has the volume fraction x_0 and the thermal conductivity K_0, the granulate materials volume fractions $x_i, 1 \leq i \leq n$ and thermal conductivities $K_i, 1 \leq i \leq n$. the average heat flow through the volume can then be calculated by the following equation:

$$\vec{\mathbf{q}}_{\mathbf{h}} = \frac{1}{V}\int_V \vec{\mathbf{q}}\, dv = \frac{1}{V}\int_V -K\vec{\mathbf{G}}\, dv \qquad (297)$$

$\vec{\mathbf{q}}_{\mathbf{h}}$	average heat flow (3D-vector) $[J\ m^{-2}\ d^{-1}]$	V	Volume of granular material $[m^3]$
$\vec{\mathbf{q}}$	local heat flow (3D-vector) $[J\ m^{-2}\ d^{-1}]$	K	local thermal conductivity $[J\ m^{-1}\ d^{-1}\ °\mathrm{C}^{-1}]$
$\vec{\mathbf{G}}$	local temperature gradient (3D-vector) $[°\mathrm{C}\ m^{-1}]$		

Assuming that throughout the volume of the same material the same temperature gradient exists, the average heat flow can be calculated by:

$$\vec{\mathbf{q}}_{\mathbf{h}} = \sum_{i=0}^{n} x_i K_i \vec{\mathbf{G}}_{\mathbf{i}} \qquad (298)$$

$\vec{\mathbf{q}}_{\mathbf{h}}$	average heat flow (3D-vector) $[J\ m^{-2}\ d^{-1}]$
K_i	thermal conductivity of material i $[J\ m^{-1}\ d^{-1}\ °\mathrm{C}^{-1}]$
x_i	volume fraction of material i [1]
$\vec{\mathbf{G}}_{\mathbf{i}}$	local temperature gradient (3D-vector)within the volume of material i $[°\mathrm{C}\ m^{-1}]$

By introducing the apparent thermal conductivity K_h $[J\ m^{-1}\ d^{-1}\ °\mathrm{C}^{-1}]$ the average heat flow $\vec{\mathbf{q}}_{\mathbf{h}}$ $[J\ m^{-2}\ d^{-1}]$ through the volume can be calculated by the average temperature gradient $\vec{\mathbf{G}}_{\mathbf{v}}$ [°C m^{-1}] within the total volume of the granular materials:

$$\vec{\mathbf{q}}_{\mathbf{h}} = -K_h \cdot \vec{\mathbf{G}}_{\mathbf{v}} \tag{299}$$

$$\vec{\mathbf{G}}_{\mathbf{v}} = \frac{1}{V} \int_V \vec{\mathbf{G}}\, dv = \sum_{i=0}^{n} x_i \vec{\mathbf{G}}_{\mathbf{i}} \tag{300}$$

and hence:

$$K_h \sum_{i=0}^{n} x_i \vec{\mathbf{G}}_{\mathbf{i}} = \sum_{i=0}^{n} x_i K_i \vec{\mathbf{G}}_{\mathbf{i}} \tag{301}$$

For the heat flow in the direction of the unit vector $\mathbf{e}$, ($\|\mathbf{e}\|$ = 1) results:

$$K_h \sum_{i=0}^{n} x_i \vec{\mathbf{G}}_{\mathbf{i}} \cdot \vec{\mathbf{e}} = \sum_{i=0}^{n} x_i K_i \vec{\mathbf{G}}_{\mathbf{i}} \cdot \vec{\mathbf{e}} \tag{302}$$

or

$$K_h = \frac{\sum_{i=0}^{n} x_i K_i \vec{\mathbf{G}}_{\mathbf{i}} \cdot \vec{\mathbf{e}}}{\sum_{i=0}^{n} x_i \vec{\mathbf{G}}_{\mathbf{i}} \cdot \vec{\mathbf{e}}} = \frac{x_0 K_0 + \sum_{i=1}^{n} f_i x_i K_i}{x_0 + \sum_{i=1}^{n} f_i x_i} \tag{303}$$

$$f_i = \frac{\vec{\mathbf{G}}_{\mathbf{i}} \cdot \vec{\mathbf{e}}}{\vec{\mathbf{G}}_{\mathbf{0}} \cdot \vec{\mathbf{e}}} \tag{304}$$

The value f_i depends on the ratio K_i/K_0 and on the size and form of the granules as well as on their relative positions within the volume.

Under the restrictions, that granules have ellipsoidal shape and, that they are so far apart that they do not interact, a mathematical expression can be given to calculate the values f_i. For a granule with principal axes a_1, a_2, a_3 the following equations for a temperature gradient in direction of the axis a_j (Burger, 1919) can be derived:

$$f_{ij} = \left[1 + (\frac{K_i}{K_0} - 1) g_j\right]^{-1} \tag{305}$$

$$g_j = \tfrac{1}{2}\, a_1 a_2 a_3 \int_0^{\infty} [(a_1^2 + u)(a_2^2 + u)(a_3^2 + u)]^{-\frac{1}{2}} (a_j^2 + u)^{-1} du \tag{306}$$

and we have

$$g_1 + g_2 + g_3 = 1 \tag{307}$$

If the ellipsoidal granulas are randomly oriented, then the factor f_i is given by the following equation (Burger, 1919):

$$f_i = \tfrac{1}{3} \sum_{j=1}^{3} f_{ij} \tag{308}$$

For a **spheroid** with axes $a_1 = a_2 = \alpha a_3$ results from equation (306):

$$\begin{aligned} g_1 &= \tfrac{1}{2}\,\alpha^2 a_3^3 \int_0^\infty [((\alpha a_3)^2 + u)^{-2}(a_3^2 + u)]^{-\frac{1}{2}}\,du \qquad (309)\\ &= \tfrac{1}{2}\,\alpha^2 \int_0^\infty (\alpha^2 + v)^{-2}(1 + v)^{-\frac{1}{2}}\,dv \\ g_2 &= g_1 \qquad (310)\\ g_3 &= 1 - g_1 - g_2 \qquad (311)\end{aligned}$$

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

$$g_1 = \tfrac{1}{2}\,\frac{\alpha^2}{(1-\alpha^2)}\Big[\frac{1}{\alpha^2} + \frac{1}{2(1-\alpha^2)^{\frac{1}{2}}}\log(\frac{1-(1-\alpha^2)^{\frac{1}{2}}}{1+(1+\alpha^2)^{\frac{1}{2}}})\Big] \qquad (312)$$

For a spherical granula $(\alpha = 1)$:

$$g_1 = \tfrac{1}{3} \qquad (313)$$

and for a prolate spheroid $(\alpha > 1)$:

$$g_1 = \tfrac{1}{2}\,\frac{\alpha^2}{(1-\alpha^2)}\Big[\frac{\pi}{2(\alpha^2-1)^{\frac{1}{2}}} - \frac{1}{\alpha^2} - \frac{1}{(\alpha^2-1)^{\frac{1}{2}}}\arctan(\frac{1}{(\alpha^2-1)^{\frac{1}{2}}})\Big] \qquad (314)$$

For all three cases:

$$g_2 = g_1 \quad \text{and} \quad g_3 = 1 - 2\,g_1 \qquad (315)$$

For **elongated cylinders with elliptical cross section**, i.e. with axes $a_1 = m\,a_2,\ m > 0$ and $a_3 = \infty$ holds:

$$g_1 = \frac{1}{m+1}, \qquad g_2 = \frac{m}{m+1}, \qquad g_3 = 0 \qquad (316)$$

For **flat particles**, with small thickness, i.e. lamellae with axes $a_2 = a_3 = \infty$ holds:

$$g_1 = 1, \qquad g_2 = g_3 = 0 \qquad (317)$$

2.2.2.2 Thermal Conductivity of Soils In the following the model presented to estimate the thermal conductivity in mixtures of granular materials shall be applied to soils. For this purpose it is assumed that soil can be considered to consist of granular material of quartz, minerals, organic matter, water, air and ice. For solid soil particles of quartz and mineral material the model of spheroidal grains is often applied using α-values out of $3,5 \leq \alpha \leq 4$ (de Vries, 1963; Hansen et al., 1990). Organic material corresponds to shapes of cylinders with elliptic cross section, i.e. to $m = 3$ in equation (316). In the following the application

of the de Vries model is described using the example of the model DAISY (Hansen et al., 1990) :
In moist soils water can be considered as continuous medium in which solid particles and air bubbles are dispersed. This often holds for the range from water saturation down to a volumetric water content, which corresponds to a matric potential that lies half way between field capacity (pF 2.53) and wilting point (pF 4.18). In dry soil, air is seen as a continuous medium. This is assumed to hold for the application of the model from air dry soil up to soil moisture at the wilting point (pF 4.2). In the range 'between soil water content half way between wilting point and field capacity, the thermal conductivity of the soil is found by interpolation' (Hansen et al., 1990).

If water is the continuous medium: In case of near water saturated soil it is assumed, that air-filled parts of the pore-space form nearly spherical air bubbles, i.e. that $\alpha = 1$ and $g_1 = g_2 = g_3 = \frac{1}{3}$. If the soil gets drier, air-filled pore-space increases, and factors f_i increase, i.e. g_1 decreases. It is further assumed, that the shapes of air-filled space resemble increasingly prolate spheroids up to a value of $\alpha = 10$ (i.e. $g_1 = 0.07$) at wilting point. By linear interpolation we obtain:

1st Case: $\frac{1}{2}(\theta_{fc} + \theta_{wp}) \leq \theta \leq \theta_{sat}$:

$$\begin{aligned} g_1 &= \tfrac{1}{3} - (\tfrac{1}{3} - 0.07)\, \frac{\theta_{sat} - \theta}{\theta_{sat} - \theta_{wp}} \\ g_2 &= g_1 \\ g_3 &= 1 - g_1 - g_2 \end{aligned} \tag{318}$$

If air is the continuous medium: For dry soil it is assumed, that air forms a continuous medium and the existing water surrounds the solid soil particles by water films, in a way that the water menisci build flat water rings at the contact areas, which form bridges for the heat flow. This will be presented by flat particles of small thickness, i.e. extended lamellae leading to:

2nd Case: $0 \leq \theta \leq \theta_{wp}$:

$$\begin{aligned} g_1 &= 1 \\ g_2 &= 0 \\ g_3 &= 0 \end{aligned} \tag{319}$$

Otherwise: If either soil water nor soil air build the dominant continuous medium, the thermal conductivities obtained from the two previous cases will be interpolated after equations (304), (306), and (309), i.e. using $\theta_{fcwp} = \frac{1}{2}(\theta_{fc} + \theta_{wp})$ we get:

3rd Case: $\theta_{wp} \leq \theta \leq \frac{1}{2}(\theta_{fc} + \theta_{wp}) = \theta_{fcwp}$:

$$K_h(\theta) = K_h(\theta_{fcwp})\, \frac{\theta - \theta_{wp}}{\theta_{fcwp} - \theta_{wp}} \; + \; K_h(\theta_{wp})\Big[1 - \frac{\theta - \theta_{wp}}{\theta_{fcwp} - \theta_{wp}}\Big] \tag{320}$$

If the soil is frozen: If the total soil water content, i.e. the volumetric content of liquid water together with the volumetric ice content is smaller than the volumetric water content at wilting point of unfrozen soil, then the thermal conductivity of unfrozen soil is also used for frozen soil. For higher total water contents the thermal conductivity of liquid water is substituted by the thermal conductivity of ice. Hereby it is assumed, that at soil frost ice replaces the heat bridges between the solid soil particles that in case of unfrozen soil are formed by liquid water.

Table 4: Thermal Parameters of Soil Materials after de Vries (1963)

Soil Constituent	ρ $kg\,m^{-3}$	c $J\,kg^{-1}\,°\mathrm{C}^{-1}$	K $J\,m^{-1}\,s^{-1}\,°\mathrm{C}^{-1}$
Quartz	2660	750	8.8
Clay-Minerals	2650	750	2.9
Organic Matter	1300	1920	0.25
Water	1000	4192	0.57
Ice	920	2050	2.2
Air	1.25	1005	0.025

ρ density $[kg\,m^{-3}]$, c specific heat capacity $[J\,kg^{-1}\,°\mathrm{C}^{-1}]$, and K heat conductivity $[J\,m^{-1}\,s^{-1}\,°\mathrm{C}^{-1}]$ of different soil materials, water and air at 10 °C (de Vries, 1963)

2.2.3 Soil Heat Transfer: Approach of the Model DAISY

Starting point for simulations of soil heat transfer by the DAISY model (Hansen et al., 1990) is equation (289), but in a reduced form as vapor flow is not considered:

$$C_h \frac{\partial T}{\partial t} - L_f \rho_i \frac{\partial \theta_i}{\partial t} = \frac{\partial}{\partial z}(K_h \frac{\partial T}{\partial z}) \; - \; \rho_w c_w \, q_w \frac{\partial T}{\partial z} \tag{321}$$

This equation is further simplified by omitting the second term of the left hand side in case no soil frost is considered. In case of a freezing soil the equation (321) is further transformed similar to the transformation presented in 2.2.1.6. For the DAISY model this is achieved using a discrete form of the Clausius-Clapeyron equation (Miller, 1980):

$$\frac{T - T_f}{T_f} = \frac{1}{L_f}\Big(\frac{\psi_m + \psi_s}{\rho_w} - \frac{p_{ice}}{\rho_{ice}}\Big), \tag{322}$$

T	soil temperature [°C]	T_f	= 273,15 °C	ψ_m	matric potential $[Pa]$
ψ_s	osmotic potential $[Pa]$	p_{ice}	ice gauge $[Pa]$	ρ_w	density of water $[kg\, m^{-3}]$
ρ_{ice}	density of ice $[kg\, m^{-3}]$	L_f	latent heat of melting $[J\, kg^{-1}]$		

In case of soil freezing or thawing the equation describes the relation between the soil matric potential, here expressed in units of energy per volume $[Pa]$, and the soil temperature. See also (Kurylyk and Watanabe, 2013) and (Dall'Amico, 2010) for different forms of the Clausius-Clapeyron equation that have been employed by various model developers.

By neglecting all other effects except the change in matric potential ψ_m we get from (322):

$$\frac{\partial T}{\partial t} = \frac{T_f}{\rho_w\, L_f} \frac{\partial \psi_m}{\partial t} = \frac{T_f}{\rho_w\, L_f} \frac{\partial \psi_m}{\partial \theta_{liq}} \frac{\partial \theta_{liq}}{\partial t} = \frac{T_f}{\rho_w\, L_f}\, C(\theta_{liq})^{-1} \frac{\partial \theta_{liq}}{\partial t} \tag{323}$$

θ_{liq}	vol. liquid water content [1]	$C(\cdot)$	differential water capacity $[Pa^{-1}]$

By using the relation $\rho_w\, \theta = \rho_w\, \theta_{liq} + \rho_{ice}\, \theta_{ice}$ and by differentiation versus time t we have

$$\frac{\partial \theta_{liq}}{\partial t} = \frac{\partial \theta}{\partial t} \; - \; \frac{\rho_{ice}}{\rho_w} \frac{\partial \theta_{ice}}{\partial t} \tag{324}$$

θ	total vol. water content [1]	θ_{liq}	vol. liquid water content [1]	θ_{ice}	vol. ice content [1]

and further inserting equation (324) into equation (323) yields:

$$\frac{\partial \theta_{ice}}{\partial t} = \frac{\rho_w}{\rho_{ice}} \Big[-\frac{\rho_w\, L_f}{T_f}\, C(\theta_{liq}) \frac{\partial T}{\partial t} + \frac{\partial \theta}{\partial t}\Big] \tag{325}$$

Assuming a zero water sink $S_w = 0$ under soil freezing conditions, the continuity equation (94) of the water flux q_w $[m\, s^{-1}]$ is inserted to get the change rate of the volumetric soil ice content (soil freezing and/or thawing rate):

$$\frac{\partial \theta_{ice}}{\partial t} = \frac{\rho_w}{\rho_{ice}} \Big[-\frac{\rho_w\, L_f}{T_f}\, C(\theta_{liq}) \frac{\partial T}{\partial t} - \frac{\partial q_w}{\partial z}\Big] \tag{326}$$

The ice forming rate is used by the DAISY water flow model under soil freezing conditions to calculate the change of the liquid water content (see section 1.7.1). This is based as for the models SHAW and SOILN on a specific form of the Clausius-Clapeyron equation.

2.2.3.1 Heat Transfer at Soil Frost By inserting equation (326) into the transport equation (321) and further transformation leads to the following heat transport equation, which is finally numerically solved by the DAISY model in case of simulating a freezing or thawing soil:

$$\Big[C_h + \frac{\rho_w^2 L_f^2}{T_f}\, C(\theta_{liq})\Big] \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}(K_h\, \frac{\partial T}{\partial z}) \; - \; \rho_w c_w\, q_w \frac{\partial T}{\partial z} \; - \; \rho_w L_f\, \frac{\partial q_w}{\partial z} \tag{327}$$

To complete the transport equation yet the initial and boundary condition have to be given:

2.2.3.2 Initial Condition To start the heat transfer simulation the initial vertical distribution of the soil temperature within the whole considered soil profile have to be given as input:

$$T(t,z) = T_0(z) \quad \text{for} \quad t = t_0, \tag{328}$$

where T_0 [°C] is a given function of the soil depth z, which represents the vertical soil temperature distribution at time t_0 $[d]$.

2.2.3.3 Upper Boundary Condition The upper boundary condition is assumed to be given by the soil temperature at the soil surface (Dirichlet boundary condition) , where the soil surface temperatures (at zero soil depth) are approximately set equal to the air temperature T_a [°C]:

$$T(t,0) = T_a \quad \text{at the soil surface} \quad z = 0 \tag{329}$$

For the air temperature T_a it is assumed, that it undergoes a diurnal cycle and reaches its maximum value at 3:00 in the afternoon, when the average daily air temperature is above that of the previous night. If the average daytime temperature is below that of the previous night, it is assumed that the minimum temperature is at 9:00 in the morning.

In case of a wet snow cover, i.e. if the snow also contains liquid water, the surface temperature T_{sur} is set to zero. In dry snow if the snow contains not much liquid water, the soil surface temperature is calculated assuming a steady state heat flow through the snow layer and the top soil:

$$-K_{h,sno}\frac{T_{sur} - T_a}{\Delta z_{sno}} = -K_{h,1}\frac{T_1 - T_{sur}}{\Delta z_1} \tag{330}$$

or resolved after T_{sur}:

$$T_{sur} = \frac{(K_{h,1}/\Delta z_1)T_1 + (K_{sno}/z_{sno})T_a}{(K_{h,1}/\Delta z_1) + (K_{sno}/z_{sno})} \tag{331}$$

K_{sno}	thermal conductivity of snow $[J\ m^{-1}\ d^{-1}\ °\mathrm{C}^{-1}]$	Δz_{sno}	height of snow cover $[m]$
T_{sur}	soil surface temperature [°C]	T_a	air temperature [°C]
$K_{h,1}$	thermal conductivity of the top soil $[J\ m^{-1}\ d^{-1}\ °\mathrm{C}^{-1}]$	Δz_1	depth of the top soil $[m]$
T_1	temperature of the topsoil [°C]		

For this purpose the thermal conductivity of the snow K_{sno} $[J\ m^{-1}\ d^{-1}\ °\mathrm{C}^{-1}]$ is determined by the following approximate formula:

$$K_{sno} = s_K\ \rho_{sno}^2\ \varphi_c \tag{332}$$

s_K = $2,86\ 10^{-6}\ J\ m^5\ s^{-1}\ °\mathrm{C}^{-1}\ kg^{-2}$ ρ_{sno} snow density $[kg\ m^{-3}]$ φ_c = $8,64\ 10^4 s\ d^{-1}$

2.2.3.4 Lower Boundary Condition If also at the bottom boundary of the soil profile a Dirichlet condition is to be applied , then a simple estimation of the temperature at the lower end of the considered soil profile is possible. Neglecting frost, thaw and convective heat transfer and assuming constant heat capacity C_h and thermal conductivity K_h of the soil, the heat transport equation reduces to::

$$\frac{\partial T}{\partial t} = \frac{K_h}{C_h}\,\frac{\partial^2 T}{\partial z^2} \tag{333}$$

This equation can be solved analytically, i.e. a closed form mathematical expression can be given, which solves the partial differential equation, if the following boundary conditions are prescribed:

$$\begin{aligned} T(t,0) &= T_{ym} + T_A \cos(\omega(t - t_0)) \quad \text{at the soil surface} \quad z = 0 && (334) \\ T(t,\infty) &= T_{ym} \quad \text{at the lower boundary of a very deep soil profile} \quad z = \infty && (335) \end{aligned}$$

The analytical solution τ of soil heat temperature [°C] is then given by:

$$\tau(t,z) = T_{ym} + T_A \exp(-z/d) \cos(\omega(t - t_0) - z/d) \quad \text{with} \quad d = \sqrt{\frac{2K_h}{C_h \omega}} \tag{336}$$

T_{ym}	annual average of air temperature [°C]	t	day in the year $[d]$
T_A	amplitude of the annual variation of air temperature [°C]	ω	= $2\pi/365$ $[d^{-1}]$
K_h	mean thermal conductivity of the soil profile $[J\ m^{-1}\ d^{-1}\ °\mathrm{C}^{-1}]$	t_0	day in the year $[d]$, when $T(t,0) = T_{ym} + T_A$
C_h	mean heat capacity of the soil profile $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$		
ℓ	depth of the soil profile $[mm]$		

By this simple estimation of the soil temperature a **lower boundary condition** can be obtained by evaluating the analytical solution for the bottom depth of the soil profile, i.e. the following Dirichlet condition can now be prescribed:

$$T(t,\ell) = \tau(t,\ell) \quad \text{at the lower edge of the soil profile} \quad z = \ell \tag{337}$$

2.2.3.5 Numerical Solution of the Heat Transport Equation According to (Hansen et al., 1990) the heat transport equation (327) used within the DAISY model is solved by applying a fully implicit finite difference scheme (s. e.g. Schwarz (1986), section 10.2.2) with the following discretization ($i,\ 1 \le i \le n$ for the space steps, and $j,\ 1 \le j \le m$ for the time steps):

$$\begin{aligned} A_i^{j+\frac{1}{2}}\,\frac{T_i^{j+1}-T_i^j}{\Delta t^{j+1}} &= (K_h)_i^{j+\frac{1}{2}}\,\frac{1}{2\,\Delta z^2}\,(T_{i+1}^{j+1}-2\,T_i^{j+1}+T_{i-1}^{j+1}+T_{i+1}^j-2\,T_i^j+T_{i-1}^j) \\ &\quad + \Big[(\frac{\partial K_h}{\partial z})_i^{j+\frac{1}{2}} - \rho_w c_w (q_w)_i^{j+\frac{1}{2}}\Big]\,\frac{(T_{i+1}^{j+1}-T_{i-1}^{j+1})-(T_{i+1}^j-T_{i-1}^j)}{4\,\Delta z} \\ &\quad - B_i^{j+\frac{1}{2}} \end{aligned} \tag{338}$$

where the superscript $j+\frac{1}{2}$ refers to values centered in time and the coefficients to:

$$A_i^{j+\frac{1}{2}} = \tfrac{1}{2}[(C_h)_i^j + (C_h)_i^{j+1}] + \frac{\rho_w^2 L_f^2}{T_0}\,C(\theta_{liq})_i^{j+\frac{1}{2}} \tag{339}$$

$$(K_h)_i^{j+\frac{1}{2}} = \tfrac{1}{2}[(C_h)_i^j + (C_h)_i^{j+1}] \tag{340}$$

$$(\frac{\partial K_h}{\partial z})_i^{j+\frac{1}{2}} = \tfrac{1}{2}\Big[\frac{(K_h)_{i+1}^{j+1} - (K_h)_{i-1}^{j+1}}{\Delta z} - \frac{(K_h)_{i+1}^{j} - (K_h)_{i-1}^{j}}{\Delta z}\Big] \tag{341}$$

$$(q_w)_i^{j+\frac{1}{2}} = \tfrac{1}{2}[(q_w)_i^j + (q_w)_i^{j+1}], \quad (q_w)_{i+\frac{1}{2}}^{j+\frac{1}{2}} = \tfrac{1}{2}[(q_w)_{i+1}^{j+\frac{1}{2}} + (q_w)_i^{j+\frac{1}{2}}] \tag{342}$$

$$B_i^{j+\frac{1}{2}} = \rho_w L_f\,\frac{(q_w)_{i+\frac{1}{2}}^{j+\frac{1}{2}} - (q_w)_{i-\frac{1}{2}}^{j+\frac{1}{2}}}{\Delta z}$$

The transformation and integration of the boundary conditions provides a tridiagonal system of equations, which is solved directly by the elimination method of Gauss (cf. 1.4.4.5).

All in all, this results in a numerical solution procedure, that allows to calculate the one-dimensional vertical temperature distribution within the soil. If no soil frost occurs, neither freezing nor thawing must be taken into account and it is then sufficient to solve the equation system for which the value of the latent heat of melting L_f equals zero.

2.2.4 Soil Heat Transfer: Approach of the Model SHAW

The ecosystem model SHAW (Flerchinger and Saxton, 1989) describes vertical soil heat transfer by the following general heat transport equation, which considers the impacts of soil frost and evaporation on the vol. heat content H $[J\ m^{-3}]$ of the soil:

$$\frac{\partial H}{\partial t} - \rho_{ice} L_f \frac{\partial \theta_{ice}}{\partial t} + L_v \left(\frac{\partial \rho_v}{\partial t} + \frac{\partial q_v}{\partial z}\right) = \frac{\partial}{\partial z}\left(K_h \frac{\partial T}{\partial z}\right) - \rho_w c_w \frac{\partial (q_w T)}{\partial z} + S_h \tag{343}$$

In the following the change of soil heat capacity is neglected, hence the change of soil heat will be given by:

$$\frac{\partial H}{\partial t} = \frac{\partial H}{\partial T}\frac{\partial T}{\partial t} = C_h \frac{\partial T}{\partial t} \tag{344}$$

2.2.4.1 Heat Transport Equation By inserting (344) into (343) results the one-dimensional soil heat transport equation, which is used by the model SHAW to simulate the dynamics of the vertical soil temperature distribution:

$$C_h \frac{\partial T}{\partial t} - \rho_{ice} L_f \frac{\partial \theta_{ice}}{\partial t} + L_v \left(\frac{\partial \rho_v}{\partial t} + \frac{\partial q_v}{\partial z}\right) = \frac{\partial}{\partial z}\left(K_h \frac{\partial T}{\partial z}\right) - \rho_w c_w \frac{\partial (q_w T)}{\partial z} + S_h \tag{345}$$

C_h	vol. soil heat capacity $[J\ m^{-3}$ °C$^{-1}]$	T	soil temperature [°C]
ρ_{ice}	density of ice $[kg\ m^{-3}]$	θ_{ice}	vol. ice content $[1]$
L_f	latent heat of phase change from solid	q_v	water vapor flux $[kg\ m^{-2}\ d^{-1}]$
	to liquid water (lat. heat of melting) $[J\ kg^{-1}]$	ρ_v	density of water vapor $[kg\ m^{-3}]$
L_v	latent heat of phase change from liquid	q_w	vol. water flux $[m\ d^{-1}]$
	to water vapor (lat. heat of vaporizaton) $[J\ kg^{-1}]$	ρ_w	density of water $[kg\ m^{-3}]$
K_h	heat conductivity of the soil $[J\ m^{-1}\ d^{-1}$ °C$^{-1}]$	c_w	specific heat capacity of water
S_h	soil heat sink or source $[J\ m^{-3}\ d^{-1}]$		$\approx\ 4200,0\ J\ kg^{-1}$ °C^{-1}

By inserting the heat conservation equation of soil water vapor flow (neglecting evaporation within the soil volume)

$$L_v\, \frac{\partial \rho_v}{\partial t} = -\, c_v\, \frac{\partial (q_v\, T)}{\partial z} \tag{346}$$

q_v	soil water vapor flux $[kg\ m^{-2}\ d^{-1}]$	c_v	specific heat capacity water vapor
	(described as mass rate)		$\approx\ 1860,0\ J\ kg^{-1}$ °C^{-1}

results the following form of the heat transport equation , which is finally solved by numerical methods:

$$C_h \frac{\partial T}{\partial t} - \rho_{ice} L_f \frac{\partial \theta_{ice}}{\partial t} + L_v \frac{\partial q_v}{\partial z} = \frac{\partial}{\partial z}\left(K_h \frac{\partial T}{\partial z}\right) - \rho_w c_w \frac{\partial (q_w T)}{\partial z} + c_v \frac{\partial (q_v T)}{\partial z} + S_h \tag{347}$$

2.2.4.2 Water Vapor Flux The water vapor flux in soil, which plays an important role in soil heat transfer, can be expressed as flux driven by a gradient in soil air humidity and a gradient of soil temperatures, cf. Campbell (1985), equation (9.9):

$$q_v = -D_v\ \rho'_v\ \frac{\partial h_r}{\partial z}\ -\ f_\eta\ D_v\ h_r\ \frac{\partial \rho'_v}{\partial T}\ \frac{\partial T}{\partial z} \tag{348}$$

q_v	water vapor flux $[kg\ m^{-2}\ d^{-1}]$	D_v	effective diffusion coefficient of soil water vapor $[m^2\ d^{-1}]$
ρ'_v	saturated water vapor density $[kg\ m^{-3}]$ at soil temperature T	h_r	relative soil air humidity $[1]$
T	soil temperature [°C]	f_η	correction factor [1]

The effective diffusion coefficient of water vapor in soil D_v $[m^2\ d^{-1}]$ is given by the diffusion coefficient of water vapor in air $D_{v,o} = 2,12\ 10^{-5}\ m^2\ s^{-1}$ and a tortuosity factor $f_{D,v} = 0,66\ \phi_{air}$ $[1]$ (Campbell, 1985), wher ϕ_{air} $[1]$ denotes the vol. fraction of the air-filled pore space, and $\varphi_c = 8,64\ 10^4\ s\ d^{-1}$ the conversion factor from days $[d]$ to seconds $[s]$:

$$D_v = D_{v,o}\ f_{D,v}\ \varphi_c \tag{349}$$

The saturated water vapor density ρ'_v $[kg\ m^{-3}]$ at soil temperature T and the slope $\partial\rho'_v/\partial T$ $[kg\ m^{-3}$ °C$^{-1}]$ and the correction factor f_η [1] according to Cass et al. (1984) are calculated by empirical equations:

$$\begin{aligned} \rho'_v &= \psi_T(T_K)\ M_w/(R\ T_K) && (350)\\ &\quad \text{with} \quad \psi_T(T_K) = \exp[52,6 - 6790,5/T_K - 5,03\log(T_K)] \quad \text{in}\ \ kPa \\ \frac{\partial \rho'_v}{\partial T} &= 1,65\ 10^{-5}\ +\ 4944,4\ \rho'_v\ T_K^{-2} && (351)\\ f_\eta &= A\ +\ B(\theta/\theta_{sat})\ - (A-D)\ \exp[-(C\theta/\theta_{sat})^E] && (352) \end{aligned}$$

T_K	soil temperature in Kelvin $[K]$	A = 9,5 B = 3,0	
M_w	molecular weight of water = 0,018 $kg\ mol^{-1}$	$C = \theta_{sat}\ (\ 1 + 2,6\ /\sqrt{f_{clay}}\ )$	
R	gas constant = 8,3143 $J\ mol^{-1}\ K^{-1}$	D = 1,0 E = 4,0	
θ	vol. water content $[1]$	f_{clay}	clay fraction of the soil $[1]$
θ_{sat}	saturated vol. water content $[1]$		

The relative humidity of soil air h_r [1] is determined from the matric potential ψ_m $[Pa]$ and the osmotic potential ψ_s $[Pa]$ of the soil, see equation (268):

$$h_r = \exp[\frac{M_w\ g}{R\ T_K}\ \frac{\psi_m + \psi_s}{\rho_w g}] \tag{353}$$

M_w	molecular weight of water = 0,018 $kg\ mol^{-1}$	g	acceleration of gravitation $= 9,81\ m\ s^{-2}$
R	gas constant = 8,3143 $J\ mol^{-1}\ K^{-1}$	ρ_w	density of water $[kg\ m^{-3}]$
T_K	soil temperature in Kelvin $[K]$		

For the description water vapor flow and its coupling with the water flow equation, i.e. the Richards equation (94), the part of water flow, which occurs due to water vapor flux is expressed as an additional sink term, such that the sink term S_w $[d^{-1}]$ of equation (94) is replaced by $\widehat{S_w}$ $[d^{-1}]$, which is defined by:

$$\widehat{S_w} = \frac{1}{\rho_w} \frac{\partial q_v}{\partial z} + S_w \tag{354}$$

q_v	water vapor flow $[kg\ m^{-2}\ d^{-1}]$	ρ_w	density of water $[kg\ dm^{-3}]$
z	soil depth $[mm]$		

2.2.4.3 Heat Conductivity of Soil The calculation of soil heat conductivity is achieved following the approach of de Vries (1963). For this purpose for each of the soil components ice, organic substance, sand, silt, clay the weighting factors f_i $[1]$ are calculated after equation (308), where it is assumed, that soil particles can be represented by spheroids:

$$f_i = \tfrac{2}{3}\left[1 + (\frac{K_i}{K_0} - 1)g_i\right]^{-1} + \tfrac{1}{3}\left[1 + (\frac{K_i}{K_0} - 1)(1 - 2g_i)\right]^{-1} \tag{355}$$

K_i	heat conductivity $[J\ m^{-1}\ d^{-1}\ °\mathrm{C}^{-1}]$ of the embedded fraction i
K_0	heat conductivity $[J\ m^{-1}\ d^{-1}\ °\mathrm{C}^{-1}]$ of the continuous fraction
g_i	form factor [1] of the embedded fraction i

Form factors are set for ice $g_i = 0,333$, for organic substance $g_i = 0,5$, for sand and silt $g_i = 0,144$ and for clay $g_i = 0,125$. The thermal conductivities K_i resp. K_0 are given by table 4, where for sand the conductivity of quartz and for silt the conductivity of clay is used.

1st Case: If $\theta \geq \theta_{dlv}$, i.e. the vol. wwater content θ $[1]$ is greater or equal to the de Vries critical value θ_{dvl} $[1]$ of water content, which is given by

$$\theta_{dvl} = 0,1 + 0,2\, f_{clay}\, (\rho_s/\rho_m) - 0,1\, f_{sand}\, (\rho_s/\rho_m) \tag{356}$$

f_{clay}	grav. clay fraction of soil [1]	f_{sand}	grav. sand fraction of soil [1]
ρ_s	bulk density of soil $[kg\ m^{-3}]$	ρ_m	density of the mineral soil fraction $[kg\ m^{-3}]$

then water is conceived as continuous medium and the heat conductivity of the enclosed soil air is determined by the form factor of soil air

$$g_i = g_{air} = 0,035 + (\theta - \theta_{dvl})/(\theta_{sat} - \theta_{dvl}) \tag{357}$$

θ_{sat}	saturated vol. water content of the soil $[1]$	θ_{dvl}	de Vries critical value of water content

using equation (355). By this factor and the form factors for the other components embedded into the soil water, and by their vol. soil fractions the thermal conductivity of the soil is determined by equation (304).

2nd Case: If $\theta < \theta_{dlv}$, it is assumed, that soil air forms the continuous medium and the thermal soil conductivity is calculated as the mean between the thermal conductivities at water content near zero and the de Vries critical value.

2.2.4.4 Heat Capacity of the Soil For the calculation of the heat capacity of the soil C_h $[J\ m^{-3}\ {}^{\circ}\mathrm{C}^{-1}]$ the model SHAW recognizes besides the contribution by the heat capacity of soil air also that due to the latent heat of evaporation:

$$\begin{aligned} C_h \;=\; & (1 - f_{Corg})\,\rho_s\,c_m \;+\; f_{Corg}\,\rho_s\,c_o \;+\; \theta_{liq}\,\rho_w\,c_w \;+\; \theta_{ice}\,\rho_{ice}\,c_{ice} \\ & +\; \phi_{air}\,\rho_{air}\,c_{air} \;+\; \phi_{air}\,L_v\,h_r\,(\frac{\partial \rho'_v}{\partial T}) \end{aligned} \tag{358}$$

f_{Corg}	gravimetric soil carbon fraction $[1]$
ρ_s	bulk density of the soil $[kg\ m^{-3}]$
c_m	specific heat capacity of the mineral soil components $[J\ kg^{-1}\ {}^{\circ}\mathrm{C}^{-1}]$
c_o	specific heat capacity of soil organic components $[J\ kg^{-1}\ {}^{\circ}\mathrm{C}^{-1}]$
θ_{liq}	vol. liquid water content $[1]$
ρ_w	density of liquid water $[kg\ m^{-3}]$
c_w	specific heat capacity of liquid water $[J\ kg^{-1}\ {}^{\circ}\mathrm{C}^{-1}]$
θ_{ice}	vol. ice content $[1]$
ρ_{ice}	density of ice $[kg\ m^{-3}]$
c_{ice}	specific heat capacity of ice $[J\ kg^{-1}\ {}^{\circ}\mathrm{C}^{-1}]$
ϕ_{air}	vol. soil air content $[1]$
ρ_{air}	density of soil air $[kg\ m^{-3}]$
c_{air}	specific heat capacity of soil air $[J\ kg^{-1}\ {}^{\circ}\mathrm{C}^{-1}]$
L_v	latent heat of phase change between liquid water and water vapor (latent heat of vaporization) $[J\ kg^{-1}]$
h_r	relative humidity of soil air $[1]$
ρ'_v	saturated density of water vapor $[kg\ m^{-3}]$ at soil temperature T
T	soil temperature [°C]

For this purpose the volumetric soil fraction ϕ_{air} $[1]$, which represents the pore volume filled with soil air and water vapor is estimated by the following equation:

$$\phi_{air} = 1 - (1 - f_{Corg})(\rho_s/\rho_m) - f_{Corg}(\rho_s/\rho_o) - \theta_{liq} - \theta_{ice} \tag{359}$$

ρ_m	density of the mineral component of the soil $[kg\ m^{-3}]$
ρ_o	density of the organic component of the soil $[kg\ m^{-3}]$

2.2.4.5 Initial and Boundary Conditions for the heat transport equation as calculated by the SHAW model can be specified by input data. Boundary conditions at the surface can also be given by simulation of heat and vapor exchange with the atmosphere, possibly additionally considering layers of straw or snow. At the lower boundary an empirical relation which includes a damping factor of soil temperature amplitudes can prescribe the bottom soil temperatures (Flerchinger and Saxton, 1989). The version of the SHAW heat transport model, which was implemented into EXPERT-N calculates the boundary conditions as described for the model DAISY. In addition the upper boundary condition can also be calculated following the approach compiled by Horton and Chung (1991), which is based on the energy balance of the heat exchange between atmosphere and soil surface, see section 2.4 and also Evett (2000).

2.2.4.6 Numerical Solution of the Heat Transport Equation For the discretisation of the transport equation a fully implicit finite difference scheme is applied and equation (347) is transformed to the following approximative form, where ($i,\ 1 \leq i \leq n$ denotes the space steps and $j,\ 1 \leq j \leq m$ the time steps):

$$\begin{aligned}
C^j_{h,i}\,\frac{T^j_i - T^{j-1}_i}{\Delta t^j} \;-\; \rho_{ice}\,L_f\,\frac{\theta^j_{ice,i} - \theta^{j-1}_{ice,i}}{\Delta t^j} + L_v\,\frac{q^j_{v,i} - q^j_{v,i-1}}{\Delta z_i} \quad &= \\
= \quad & \frac{\widetilde{K}^j_{i+\frac{1}{2}}\,(T^j_{i+1} - T^j_i) - \widetilde{K}^j_{i-\frac{1}{2}}\,(T^j_i - T^j_{i-1})}{\frac{1}{2}(z_{i+1} - z_{i-1})} \\
& - \rho_w\,c_w\,\frac{q^j_{w,i}\,T^j_{i+1} - (q^j_{w,i} + q_{w,i-1})\,T^j_i + q^j_{w,i-1}\,T^j_{i-1}}{\frac{1}{2}(z_{i+1} - z_{i-1})} \\
& + c_v\,\frac{q^j_{v,i}\,T^j_{i+1} - (q^j_{v,i} + q_{v,i-1})\,T^j_i + q^j_{v,i-1}\,T^j_{i-1}}{\frac{1}{2}(z_{i+1} - z_{i-1})} \\
& + S_{h,i}
\end{aligned} \tag{360}$$

with abbreviations

$$\widetilde{K}^j_{i+\frac{1}{2}} = \frac{\sqrt{K^j_{i+1}\,K^j_i}}{\Delta z_i}\ ,\ \Delta z_i = z_i - z_{i-1}\ \text{und}\quad \Delta t^j = t^j - t^{j-1} \tag{361}$$

From this form results a non-linear tridiagonal system of equations, which is solved by use of a Picard iteration (cf. section 1.4.4.6) and the elimination method of Gauss (cf. 1.4.4.5).

2.2.5 Soil Heat Transfer: Approach of the Model SOILN

In the model SOILN (Jansson and Halldin, 1980; Jansson, 1999) soil heat transfer is simulated based on the following general balance equation of heat fluxes:

$$\frac{\partial H}{\partial t} - \rho_{ice} L_f \frac{\partial \theta_{ice}}{\partial t} = \frac{\partial}{\partial z}\left(K_h \frac{\partial T}{\partial z}\right) - \rho_w c_w \frac{\partial (q_w\, T)}{\partial z} - L_v \frac{\partial q_v}{\partial z} + S_h \tag{362}$$

H	vol. heat content of the soil $[J\ m^{-3}]$	T	soil temperature [°C]
ρ_{ice}	density of ice $[kg\ m^{-3}]$	θ_{ice}	vol. ice content [1]
L_f	latent heat of phase change between ice and liquid water (latent heat of melting) $[J\ kg^{-1}]$	q_v	water vapor flux $[kg\ m^{-2}\ d^{-1}]$
		S_h	source or sink of soil heat $[J\ m^{-3}\ d^{-1}]$
L_v	latent heat of phase change of liquid water to vapor (latent heat of vaporization) $[J\ kg^{-1}]$	q_w	vol. water flux $[m\ d^{-1}]$
		ρ_w	density of water $[kg\ m^{-3}]$
K_h	thermal conductivity of soil $[J\ m^{-1}\ d^{-1}\ °\text{C}^{-1}]$	c_w	heat capacity of water $[J\ kg^{-1}\ °\text{C}^{-1}]$

This equation is not used by the model SOILN in the sense of a partial differential equation, but instead for each numerical soil layer the heat fluxes are calculated and balanced in every time step, whereby the convective terms, in which water and vapor fluxes occur are neglected. From the resulting soil heat content of each numerical soil layer its soil temperature is calculated. This numerical method almost corresponds to a forward solution of the transport equation (362) applying a method of lines approach (**?**).

Initial and boundary conditions are specified as described in the section about the model DAISY .

2.2.5.1 Unfrozen Soil For an unfrozen soil the heat capacity C_h $[J\ m^{-3}\ °\text{C}^{-1}]$ can be obtained directly from equation (285) as the soil temperature T_i results for each numerical layer $0 \le i \le n$ from the vol. heat content H_i of this layer and the defining relation $H_i = C_{h,i} T_i$ of heat capacity.

In SOILN the thermal conductivity or heat conductivity K_h $[J\ m^{-1}\ d^{-1}\ °\text{C}^{-1}]$ of the mineral soil is directly determined by using the following approach according to Kersten (1949):

$$K_h = \max\{0,05;\ a_1\ 10^{a_2 \rho_s}\ [a_3 + a_4 \log_{10}(\theta/\rho_s)]\} \tag{363}$$

ρ_s	soil bulk density $[kg\ m^{-3}]$	θ	vol. soil water content [1]
a_1	=0,1443	a_2, a_3, a_4	empirical constants [1]

The thermal conductivity of a humus layer is estimated according to Campbell (1985), p.33:

$$K_h = h_1\ +\ h_2\, \theta \tag{364}$$

θ	vol. water content of the humus layer [1]	h_1=0,06	h_2=0,74

2.2.5.2 Frozen Soil For the description of heat propagation in a frozen soil, it is assumed, that the freezing point depression can be expressed by a simple functional relationship and that the interface between iced and liquid water behaves in analogy to the interface between liquid and vapor water, i.e. the unfrozen water below zero degree can also be set in relation to a soil matric potential and to an unsaturated hydraulic conductivity.
It is further assumed, that at a soil temperature T_f below -5°C the total soil water is frozen with the exception of an small amount of residual liquid water. This residual water content of unfrozen water θ_{lf} [1] is estimated using a constant d_1 [1] and the water content at wilting point θ_{wp}, i.e. at a matric potential of pF 4.2:

$$\theta_{lf} = d_1 \, \theta_{wp} \tag{365}$$

At temperatures below T_f heat transport and temperature distribution are calculated analogously to unfrozen soil. If, however the soil temperature T is below 0 °C and above T_f, the vol. heat capacity of the soil $C_{h,f}$ $[J\ m^{-3}\ °\mathrm{C}^{-1}]$ is calculated according to equation (286):

$$C_{h,f} = \rho_m c_m (1-\phi) + \rho_w c_w \theta_{lf} + \rho_{ice} c_{ice} \theta_{ice} \tag{366}$$

ϕ	soil porosity [1]	θ_{lf}	vol. residual unfrozen water content [1]
θ_{ice}	vol. ice content [1]	ρ_m	density of the mineral soil compounds $[kg\ m^{-3}]$
c_m	specific heat capacity of the mineral soil compounds $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$		
ρ_w	density of liquid water $[kg\ m^{-3}]$	c_w	specific heat capacity of liquid water $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$
ρ_{ice}	density of ice $[kg\ m^{-3}]$	c_{ice}	specific heat capacity of ice $[J\ kg^{-1}\ °\mathrm{C}^{-1}]$

where the related vol. ice content θ_{ice} results from the vol. total water content θ:

$$\theta_{ice} = \frac{\rho_w}{\rho_{ice}} (\theta - \theta_{lf}) \tag{367}$$

This results in the corresponding vol. soil heat content H_f $[J\ m^{-3}]$ at soil temperature T_f:

$$H_f = C_{h,f} T_f - \rho_{ice} L_f \theta_{ice} \tag{368}$$

and the following ratio of latent heat of ice to heat content of soil H_f:

$$f_l = \frac{\rho_{ice} L_f \theta_{ice}}{H_f} \tag{369}$$

The freezing point depression can then be expressed by the ratio of heat content H at soil temperature T with 0 °C $> T > T_f$ and the heat content H_f at soil temperature T_f:

$$f_r = \Big(1 - \frac{H}{H_f}\Big)^{d_2 \lambda + d_3} \min\Big(1;\ \frac{H_f - H}{H_f + \rho_{ice} L_f \theta_{ice}}\Big) \tag{370}$$

λ	Brooks and Corey exponent [1], s. eq. (109)	d_2, d_3	empirical constants [1]

The vol. content of sensible heat H_s $[J\ m^{-3}]$ is given by

$$H_s = H\ (1 + f_l)\ (1 - f_r) \tag{371}$$

from which finally the soil temperature is obtained as a function of sensible heat content:

$$T = \frac{H_s}{C_{h,f}} \tag{372}$$

The calculation of the thermal conductivity $K_{h,f}$ $[J\ m^{-1}\ d^{-1}\ °\text{C}^{-1}]$ of a fully frozen soil follows the approach of Kersten (1949):

$$K_{h,f} = b_1\ 10^{b_2 \rho_s}\ +\ b_3\ 10^{b_4 \rho_s} (\theta / \rho_s) \tag{373}$$

ρ_s	soil bulk density $[kg\ m^{-3}]$	θ	vol. soil water content $[1]$
b_1, b_2, b_3, b_4	empirical constants $[1]$		

At soil temperatures between 0 °C and T_f a weighted thermal conductivity $K_{h,g}$ $[J\ m^{-1}\ d^{-1}\ °\text{C}^{-1}]$ is calculated:

$$K_{h,g} = f_q\ K_{h,f} + (1 - f_q) K_h \tag{374}$$

where f_q [1] denotes the thermal quality, i.e. the mass ratio of frozen to liquid water:

$$f_q = \min(1; -\frac{H - H_s}{\rho_{ice} \theta_{ice} L_f}) \tag{375}$$

For the fully frozen humus layer the additional impact of frozen water on the thermal conductivity is reckognized by:

$$K_{h,f} = [1\ +\ 2\ f_q\ (\theta / 100)^2]\ K_h \tag{376}$$

2.2.5.3 Water Vapor Flux The water vapor flux between two adjacent numerical soil layers is calculated by considering the water vapor gradient and the effective diffusion coefficient of water vapor. The effective coefficient of diffusion is composed by the diffusion coefficient of water vapor in free air $D_{v.o}$ $[m^2\ s^{-1}]$ and the tortuosity factor $f_{D,v}$ [1], which expresses the deviation from free diffusion caused by the narrow pore spaces. Hence the water vapor flow q_v $[kg\ m^{-2}\ d^{-1}]$ is given by:

$$q_v = -\phi_{air}\ f_{D,v}\ D_{v.o} \varphi_c\ \frac{\partial c_v}{\partial z} \tag{377}$$

where φ_c denotes the conversion factor $8,64\ 10^4\ s\ d^{-1}$.

The diffusion coefficient $D_{v.o}$ $[m^2\ s^{-1}]$ is expressed as function of soil temperature T [°C]:

$$D_{v,o} = \Big(\frac{T + 273,16}{273,16}\Big)^{1,75} \tag{378}$$

The water vapor concentration c_v $[kg\ m^{-3}]$ is determined by the soil temperature T [°C] and the vapor pressure e_v $[Pa]$ within the soil:

$$c_v = \frac{M_w\ e_v}{R\ (T + 273,16)} \tag{379}$$

M_w molecular weight of water $= 0,018\ kg\ mol^{-1}$

R gas constant $= 8,3143\ J\ mol^{-1}\ K^{-1}$,

where the water vapor pressure itself depends on the soil matric potential h $[m]$ and the soil temperature T [°C], see also eq. (351):

$$e_v = e_s\ \exp\Big[\frac{-h\ M_w\ g}{R\ (T + 273,16)}\Big] \tag{380}$$

e_s saturated water vapor pressure $[Pa]$

g acceleration of gravity $= 9,81\ m\ s^{-2}$

The coupling of the equation of water vapor flow to the water flow equation is achieved in a way similar to the model SHAW by extending the appropriate sink terms, see again equation (354) which extends the sink term of the Richards equation.

2.2.6 Soil Heat Transfer: Approach of the Model LEACHN

The simulation of heat transfer and soil temperatures, as it is achieved by the model LEACHN, follows the approach of Tillotson et al. (1980). Basis for the simulations is the heat tranfer or heat transport equation

$$C_h \, \frac{\partial T}{\partial t} \; = \; \frac{\partial}{\partial z}[\, K_h \frac{\partial T}{\partial z} \,] \tag{381}$$

$T = T(t, z)$	soil temperature [°C]
K_h	thermal or heat conductivity of the soil $[J \; m^{-1} \; d^{-1} \; ^\circ \; \mathrm{C}^{-1}]$
C_h	volumetric Heat capacity of the soil $[J \; kg^{-1} \; ^\circ\mathrm{C}^{-1}]$

The volumetric heat capacity of the soil C_h results from

$$C_h = \rho_s \, c_s \, (1 - \phi) \; + \rho_w \, c_w \, \theta \tag{382}$$

ρ_s	density of solid soil $[kg \; dm^{-3}]$	θ	vol. soil water content [1]
ϕ	soil porosity [1]	ρ_w	density of water (= 1,0 $kg \; dm^{-3}$)
c_s	specific heat capacity of solid soil (=0,84 $kJ \; kg^{-1} \; ^\circ\mathrm{C}^{-1}$)		
c_w	specific heat capacity of water (= 4,2 $kJ \; kg^{-1} \; ^\circ\mathrm{C}^{-1}$)		

The equation of heat transfer is numerically solved almost in the same way as the solute transport-equation (see 3.1.1). The upper boundary condition is given by interpolating the average weakly air temperature and the average weakly temperature amplitude. The temperature at the soil surface increases linearly from a daily minimum temperature at 6 o'clock to a daily maximum at 14:24 o'clock (60% of the day, and the decreases linearly until 21:00 o'clock, to a temperature, which is 30% of the actual temperature range above the minimal daily temperature $T = 0,3 \; (T_{max} - T_{min}) + T_{min}$. The minimal temperature is then reached by further linear temperature decrease until 6:00 o'clock of the next day. The lower boundary condition is determined by prescribing the temperature of a heat reservoir. To this end it is assumed (only for the heat transport), that the lowest soil layer has a thickness 2 m and there occurs no heat flux across the lower boundary at this depth. This leads to a high heat capacity for the lowest numerical soil layer and a more distinct temperature lag at the lower boundary.

2.3 Soil Temperature Simulation: Approach of the Model CERES

The procedure to simulate soil temperatures used by the model CERES is adapted from the approach applied by the EPIC-model (Williams et al. 1984). The calculation of the soil temperature at the soil surface T_s is performed by

$$T_s = (1,0 - \alpha_s)[0,5(T_{min} + T_{max}) + 0,5(T_{max} - T_{min})\sqrt{0,03\ R_g}] + \alpha_s T_g \qquad (383)$$

α_s	soil albedo [1]
T_{min}	minimal daily air temperature [°C]
T_{max}	maximal daily air temperature [°C]
R_g	global daily radiation $[MJ\ m^{-2}\ d^{-1}]$
T_g	moving average of soil surface temperature [°C] of the last 5 days

To simulate the soil temperature at different soil depths, the soil depth z_T is calculated, at which soil temperature is almost not affected by the daily fluctuation of air temperature. This soil depth, which is is known as the damping depth of soil temperature , results from

$$z_T = a_T\ \exp\{b_T\ [(1,0 - c_T)/(1,0 + c_T)]^2\} \qquad (384)$$

a_T	$= 1000,0 + 2500,0\ \rho_m/[\rho_m + 686,0\ \exp(-5,63\ \rho_m)]$
b_T	$= \ln(500,0/a_T)$
c_T	$= [\sum_i(\theta_i - \theta_{pwp,i})\ d_i]/(\zeta\ \sum_i\ d_i)$
ζ	$= 0,356 - 0,144\ \rho_m$
θ_i	actual vol. water content of the i-th soil layer
$\theta_{pwp,i}$	vol. water content at permanent wilting point of the i-th soil layer
ρ_m	average bulk density $[kg\ dm^{-3}]$ of the total soil profile
d_i	thickness of the i-th soil layer $[mm]$

The daily average soil temperature of the i-th soil layer T_i [°C] is finally estimated as follows:

$$T_i = T_{ym} + [0,5\ T_A \cos(\tau + z_T/D_i) + (T_{ym} + 0,5\ T_A \cos(\tau) - T_g)] \exp(z_T/D_i) \qquad (385)$$

T_{ym}	yearly average of air temperature [°C]
T_A	yearly temperature amplitude [°C] of the monthly air temperature averages of the site
τ	= $(t_{day} - 200)2\pi/365$ gives a relation between the actual day of the year t_{day} and the hottest day of the year, which occurs at the northern hemisphere around the 20th of July(=200th day of the year)
D_i	=$\sum_j^i d_j$ [mm] depth of the lower boundary of the i-th soil layer

2.4 Energy Balance at the Soil Surface

From the energy balance at the soil surface we can calculate the energy partitioning at the soil surface and hence the soil surface temperature, which then gives the upper boundary condition (of Dirichlet type) for the soil heat transport equation.

At the soil surface three major mechanisms, radiation, convection, and conduction are simultaneously responsible for the heat transfer into the soil. Radiative heat transfer includes incoming direct and diffusive short wave solar radiation R_s $[MJ\ m^{-2}\ d^{-1}]$, longwave sky radiation R_l $[MJ\ m^{-2}\ d^{-1}]$ to the soil surface, and longwave radiation outward from the soil surface R_h $[MJ\ m^{-2}\ d^{-1}]$. Further heat fluxes that have to be to be considered are the soil heat flux from the soil surface into the soil (positive downward) G $[MJ\ m^{-2}\ d^{-1}]$, and the fluxes of latent heat LE $[MJ\ m^{-2}\ d^{-1}]$ by soil evaporation (positive upward) and of sensible heat (positive upward) H_s $[MJ\ m^{-2}\ d^{-1}]$ (Horton and Chung, 1991; Sonntag et al., 1995; Bachmann, 1998; Evett, 2000).

The exchange of energy at the soil surface is then described by the following energy balance equation:

$$R_n\ -\ H_s\ - LE\ -\ G\ =\ 0 \tag{386}$$

where R_n $[MJ\ m^{-2}\ d^{-1}]$ denotes the net-radiation absorbed by the soil at the soil surface.

Net-Radiation The net-radiation R_n $[MJ\ m^{-2}\ d^{-1}]$ itself results then from:

$$R_n = R_{n_s} + R_{n_l} = (1 - \alpha_s)\ R_g\ +\ (R_l\ -\ R_h) \tag{387}$$

The shortwave net-radiation R_{n_s} $[MJ\ m^{-2}\ d^{-1}]$ is determined by the daily incoming global radiation R_g $[MJ\ m^{-2}\ d^{-1}]$ and the albedo of the soil α_s [1], see also equation (17) and (40). The longwave net radiation R_{n_l} $[MJ\ m^{-2}\ d^{-1}]$ results from the difference between absorbed longwave radiation from the atmosphere R_l $[MJ\ m^{-2}\ d^{-1}]$ and longwave radiation R_h $[MJ\ m^{-2}\ d^{-1}]$ outward from the soil surface.

In the case of vegetation, the global radiation R_g, which hits the soil is estimated from the global radiation measured above the vegetation cover $\widetilde{R_g}$ $[MJ\ m^{-2}\ d^{-1}]$ using an exponential term, which considers the extinction of the global radiation by the leaf layers:

$$R_g = \widetilde{R_g}\exp(-f_{ext}\ f_{LAI}) \tag{388}$$

f_{ext}	= 0,49 extinction coefficient [1]	f_{LAI}	leaf area index [1]

From the amount of global radiation which hits the soil surface R_g we can estimate the absorbed shortwave radiation by use of the soil albedo α_s [1], see equation (17). To this end the soil albedo is calculated following van Bavel and Hillel (1976) in depndenc of the vol.

soil water content θ [1] at the soil surface:

$$\alpha_s = \begin{cases} 0,25 & \text{for } \theta \leq 0,10 \\ 0,35 - \theta & \text{for } 0,10 < \theta \leq 0,25 \\ 0,10 & \text{for } 0,25 < \theta \end{cases} \tag{389}$$

To estimate the rhe longwave sky irridiance, the atmosphere as a whole is approximatively seen gray radiator with emissivity ϵ_a [1] radiating at air temperature T_a. This longwave radiation from the atmosphere $\widetilde{R_l}$ $[MJ\ m^{-2}\ d^{-1}]$ is then determined by the Stefan-Boltzmann law:

$$\widetilde{R_l} = \epsilon_a\ \sigma\ (T_a + 273,16)^4 \tag{390}$$

ϵ_a	emissivity of the atmosphere [1]	σ	Stefan-Boltzmann constant = $4,9\ 10^{-9} MJ\ m^{-2} d^{-1} K^{-4}$

The part of $\widetilde{R_l}$, which is then absorbed by the soil corresponds to the emission capacity of the soil, since the soil can be regarded as almost a black body and the absorption properties of a black body correspond precisely to the emission properties. In other words, it applies to the absorbed long-wave radiation content R_l, if ϵ_s [1] denotes the soil emissivity:

$$R_l = \epsilon_s\ \widetilde{R_l} = \epsilon_s\ \epsilon_a\ \sigma\ (T_a + 273,16)^4 \tag{391}$$

The emissivity of the atmosphere ϵ_a can be calculated from a modified formula of Brunt (van Bavel and Hillel, 1976), and the emissivity of the soil ϵ_s following Horton (1989):

$$\epsilon_a = 0,605 + 0,048\ \sqrt{h_a\ e_s} \tag{392}$$

$$\epsilon_s = 0,9 + 0,08\ (\theta/\theta_{sat}) \tag{393}$$

h_a	relative air humidity [1]	e_s	saturation pressure of the air $[kPa]$, s. eq. (355)
θ	vol. soil water content [1]	θ_{sat}	saturated vol. water content [1]

Finally, the longwave radiation R_h, which the soil emits at the soil surface in dependence of the soil surface temperature T_s is calculated per surface unit as follows:

$$R_h = \epsilon_s \sigma (T_s + 273,16)^4 \tag{394}$$

Latent heat of evaporation According to Horton et al. (1984) the exchange of latent heat LE $[MJ\ m^{-2}\ d^{-1}]$ can be determined by:

$$LE = \rho_a\ c_a \frac{h_s\ e_s\ -\ e_a}{\gamma\ r_a} \tag{395}$$

ρ_a	density of air $[kg\ m^{-3}]$	c_a	specific heat capacity of the air $[MJ\ kg^{-1}\ K^{-1}]$
h_s	rel. humidity of soil air [1]	e_s	saturation vapor pressure of the air $[kPa]$
e_a	vapor pressure of the air $[kPa]$	γ	psychrometric constant $[kPa\ K^{-1}]$
r_a	aerodynamic resistance $[d\ m^{-1}]$		

Additionally the aerodynamic resistance r_a $[d\ m^{-1}]$ can be calculated using equation (29) and the psychrometric constant γ $[kPa\ K^{-1}]$ by equation (36):

$$\gamma = \frac{M_a\ c_a\ p_a}{M_w\ L^*} \tag{396}$$

M_a	molecular weight of air $[g\ mol^{-1}]$	M_w	molecular weight of water vapor $[g\ mol^{-1}]$
c_a	specific heat capacity of air $[MJ\ kg^{-1}\ K^{-1}]$	L^*	latent heat of vaporation $[MJ\ kg^{-1}]$
p_a	atmospheric air pressure $[kPa]$		

Assuming that the water vapor-air mixture behaves like an ideal gas and, since the partial water vapor pressure is much lower than the air pressure, the ideal gas law applies, i.e. according to equation (37):

$$\rho_a = \frac{M_a\ p_a}{R\ (T_a + 273{,}16)} \tag{397}$$

ρ_a	density of air $[kg\ m^{-3}]$	M_a	molecular weight of air $[g\ mol^{-1}]$
p_a	atmospheric air pressure $[kPa]$	R	universal gas constant $= 8{,}314\ J\ mol^{-1}\ K^{-1}$
T_a	air temperature [°C]		

The corresponding relationship is obtained between the density of the air in the soil, the air pressure prevailing in the soil and the soil temperature. From this and from the approximation for the vapor pressure of the air $e_a = h_a\ e_s(T_a)$ $[kPa]$ results an equation for the latent heat flow LE as a function of air and soil temperature T_a and T_s and of relative humidity of air and soil air h_a and h_s:

$$\begin{aligned} LE &= \rho_a\ c_a\ \frac{h_s\ e_s(T_s)}{\gamma\ r_a} - \rho_a\ c_a\ \frac{h_a\ e_s(T_a)}{\gamma\ r_a} \\ &= \frac{L^*\ M_w}{r_a\ R}\left(\frac{h_s\ e_s(T_s)}{T_s + 273{,}16} - \frac{h_a\ e_s(T_a)}{T_a + 273{,}16}\right) \end{aligned} \tag{398}$$

The relative soil air humidity h_s is determined from the soil matric potential h $[m]$ and the soil temperature T_s [°C] (Horton et al., 1984; Hanks and Ashcroft, 1980; Horton and Chung, 1991):

$$h_s = \exp[\frac{h}{46{,}97\ (T_s + 273{,}16)}] \tag{399}$$

The volumetric latent heat of vaporation L $[MJ\ m^{-3}]$ of water ($L = \rho_w\ L^*$, ρ_w density of water $[kg\ m^{-3}]$) is given by the parametrisation following Horton et al. (1984):

$$L = 2494{,}63 - 2{,}247\ T_s \tag{400}$$

The saturated water vapor pressure of the air e_s $[kPa]$ is calculated as function of the temperature of air T [°C] or soil air after Horton et al. (1984), cf. also equation (14) resp.(32):

$$e_s(T) = 0,611\ \exp(\frac{17,27\,T}{237,3\ +\ T}) \tag{401}$$

Sensible Heat The flux of sensible heat H_s $[MJ\ m^{-2}\ d^{-1}]$ can be calculated following Horton et al. (1984); Horton and Chung (1991) from the difference between air temperature T_a [°C] and soil temperature T_s [°C] , if it is assumed, that the air density ρ_a $[kg\ m^{-3}]$ and the specific heat capacity of the air c_a $[MJ\ kg^{-1}$ °C$^{-1}]$ are constant and known and the aerodynamic resistance r_a behaves the same during the transport of latent and sensible heat :

$$H_s = \rho_a\, c_a\, \frac{T_s - T_a}{r_a} \tag{402}$$

Soil heat flux The soil heat flux G $[MJ\ m^{-2}\ d^{-1}]$ at the soil surface can be understood (similar to the calculation of the lower boundary condition of soil heat transfer) simply as being caused by pure heat conduction (Horton, 1989):

$$G = -K_h\, \frac{\partial T}{\partial z}\bigg|_{z=0} \tag{403}$$

K_h	thermal conductivity of the soil $[MJ\ m^{-1}\ d^{-1}$ °C$^{-1}]$
$\frac{\partial T}{\partial z}\big\vert_{z=0}$	temperature gradient at the soil surface [°C m^{-1}]

and can then be estimated by an approximation of the equation describing the heat flux by heat conduction (Horton and Chung, 1991):

$$G\ \approx\ -\ K_{h,1}\left(\frac{T_2 - T_s}{\Delta z}\right)\ +\ (T_s - T_1)\, C_{h,1}\ \Delta z/(2\Delta t) \tag{404}$$

T_s	Temperature at the soil surface [°C]	Δz	vertical space step $[m]$	Δt	time step $[d]$
$K_{h,1}$	thermal conductivity of the upper soil horizon $[MJ\ m^{-1}\ d^{-1}$ °C$^{-1}]$				
T_1	Temperature at the soil surface at previous time step [°C]				
T_2	Temperature of the upper most soil layer at previous time step [°C]				
$C_{h,1}$	vol. heat capacity of the uppermost soil layer $[MJ\ m^{-3}$ °C$^{-1}]$				

Resulting temperature at the soil surface By inserting equations (388) -(404) the energy balance equation (387) results in a nonlinear equation for the soil surface temperature T_s. This equation is solved using a bisection method to calculate zeros (Horton and Chung, 1991) and by this the temperature T_s. The surface temperature of the soil thus determined can then be used as the upper boundary condition (Dirichlet condition) for the soil heat transport equation.

3 Soil Nitrogen: Transport and Transformation

3.1 Introduction

As a growth limiting factor nitrogen (N) plays an decisive role in agricultural plant production, although compared to carbon (C), hydrogen (H) and oxygen (O) it is only a minor constituent of living matter. Yet nitrogen is required in the composition of the bio-molecules DNA and RNA that contain the genetic information. It is also vital in proteins providing messengers, receptors, catalysts and structural components of cells and membranes. But whereas the major elements C, H, and O can be captured by plants from huge natural reservoirs in form of carbon dioxide (CO_2) and water H_2O, the bimolecular N which makes up 79% of the atmosphere can not be used or synthesized by the majority of organisms. Animals and humans consume N by feeding on plant tissues where N has been fixed. But plants can not fix the atmospheric N either, they take up N mostly in form of ammonia (NH_4^+) or nitrates (NO_3^-) dissolved in soil water.

An important source for these plant available N-forms is the N-fixation, i.e. the transformation of bimolecular nitrogen (N_2) into the chemically reactive compound ammonia (NH_4^+). Most natural N-fixation is done by certain bacteria that live in the soil or in the nodules on the roots of leguminous plants (i.e. beans, peas, clover, acacia trees). Another natural source is the N-mineralisation or ammonification, a process that results from the decomposition of organic matter carried out by aerobic and anaerobic bacteria. Other bacteria transform the ammonia (NH_4^+) further into nitrites (NO_2^-) and then into nitrates (NO_3^-), a process known as nitrification.

Under oxygen-poor conditions nitrates (NO_3^-) can be reduced by bacteria to gaseous nitrous oxide (N_2O) or bimolecular nitrogen (N_2) and thus are transformed into forms of nitrogen that cannot be taken up by plants. Another loss occurs during infiltration e.g. caused by heavy rainfall, when nitrates are transported below the rooted soil zone into the groundwater, i.e. beyond the reach of the plants. Because of these natural losses the plant available N often is not sufficient for optimal plant growth.

Traditional (and pre-industrial) farmers tried to replace natural N losses and N withdrawal due to their crop harvests by enriching their soils with organic matter of crop residues or of animal and human wastes. They also cultivated leguminous crops to enrich the soils with nitrogen taken up from the atmosphere by N-fixing bacteria. In some cases they ploughed these crops completely into the soil without harvesting food from them (green manure). Yet even this practice did not break the constraints of the nitrogen cycle.

Only the invention of the technical N fixation, i.e. the ammonia synthesis from nitrogen (N_2) and hydrogen (H_2) by the Haber-Bosch process and its subsequent commercialisation made N fertilizers available almost in an unlimited way and resulted in breaking through the natural nitrogen barrier of agricultural crop production (Smil, 1997). The application of synthetic N fertilizers nowadays ensures the human survival in a number of land-scarce countries with high population densities, but the massive input of reactive nitrogen into soils by industrial farming also lead to environmental pollution and problems ranging 'from local health to global changes and extends from deep underground to high in the atmosphere' (Smil, 1997).

The massive input of reactive N-compounds into agricultural soils most often leads to
(i) groundwater pollution by leaching of high amounts of nitrate,
(ii) eutrophication of nearby surface waters as ponds and lakes,
(iii) increased soil acidification and
(iv) high nitrous oxide (N_2O) emissions into the atmosphere, where N_2O contributes to the depletion of the stratospheric ozone layer (a layer that screens out dangerous ultraviolet light) and promotes green house warming in the troposphere (Fabian, 2002).

And whereas N-depositions that bring back N-compounds released to the atmosphere can have beneficial fertilizing effects, higher doses may overload sensitive ecosystems as observed in some forest systems (Nihlgard, 1985).

A promising way to reduce the worldwide growth in nitrogen use is in developing more efficient methods to fertilize crops. A fertilisation, that is directly oriented at the N-demand of the crop and continuously adapted to the plant available mineral N in soils, helps to avoid environmental pollution.

An important contribution to a more accurate estimation of the soil mineral N pool size is by numerical simulation of the complete agro-ecosystem N-cycle that also considers local soil variability and actual soil moisture conditions to optimize the timing of fertilizer applications (Booltink et al., 2001).

3.2 N-Transport

3.2.1 Equations of Nitrogen Transport in Soils

Solute transport through the soil matrix is mainly determined by two transport processes, by **molecular diffusion** due to a concentration gradient of the substance in soil solution or in soil air and by **convection** of the substance as result of the flow of soil water, in which the substance is solved or by the flow of air in which the substance is present. The movement of water around the solid phase of the porous soil matrix causes transport effects due to **dispersion**, which is mathematically described similar to molecular diffusion. Therefore, the effective dispersion is usually defined in a way that it includes molecular diffusion and also takes into account time delays along and mixing rates between different flow paths of the water. Since the geometry and the volume fraction of the water-filled pore space can strongly change during water flow in unsaturated soil, the associated solute transport is usually a very complex process. In particular at high water flow velocities, it is still only poorly understood (Roth, 1996).

If the water flows slowly enough, it is often possible to describe solute transport with sufficient accuracy, if it is assumed that the solute concentrations in different pore spaces within a small soil volume do not differ significantly from each other and the dispersion coefficient can be described by a constant value for the dispersivity independent of water flow (Roth, 1996). In this simple case, solute transport in the soil can be simulated by use of the equations for water flow and mass transport.

In addition, we will describe the phase transitions of the substance between the dissolved phase in soil water, the so-called liquid phase, and the phase bound to the soil matrix, the so-called solid phase, and transitions between the liquid phase and the gaseous phase. In the following this will be done under the simplifying assumption, that the phases, the dissolved and the solid or the dissolved and the gaseous phase are in direct equilibrium with each other.

Furthermore, the **sources and sinks**, which exist in the soil volume have to be considered for the respective substance, in order to describe transformation, degradation, or root uptake of the substance under consideration. Source and sink terms can also represent the coupling between different solute transports, e.g. the exchange of nitrogen species due to nitrification or nitrate ammonification during transport of ammonium and nitrate. Especially for the simulation of nitrate transport the process of N-mineralisation and the accompanying processes of nitrification and denitrification are important. Since these processes are closely linked to soil C-mineralisation and soil C-turnover, the description of N-transport depends also on the description of soil C-transformations.

3.2.1.1 Mass concentration and flux concentration For the mass ΔM_I $[kg]$ of a substance I in a sufficiently small cube-shaped soil volume with the edge length Δz $[m]$ the **mass concentration** c_I $[kg\ m^{-3}]$ is defined as follows

$$c_I = \frac{\Delta M_I}{\Delta z^3} \tag{405}$$

The 'sufficiently small' property should ensure that the volume of the soil in terms of the distribution of the substance I is well mixed, i.e. that there are no significant mass differences between different sites within this soil volume. Therefore then a differential description of mass concentration and hence of mass transport dynamics is possible.

Accordingly, the mass concentration $c_{I,w}$ $[kg\ m^{-3}]$ in the liquid phase and the mass concentration $c_{I,a}$ $[kg\ m^{-3}]$ in the gaseous phase are defined by:

$$c_{I,w} = \frac{\Delta M_{I,w}}{\theta\ \Delta z^3} \qquad \text{and} \qquad c_{I,a} = \frac{\Delta M_{I,a}}{\eta\ \Delta z^3} \quad , \tag{406}$$

where $\Delta M_{I,w}$ $[kg]$ denotes the mass of the substance I dissolved in soil water and $\Delta M_{I,a}$ $[kg]$ the mass of the substance I within soil air. θ [1] is the vol. water content and η [1] the vol. air content of the considered soil volume.

For the definition of the mass concentration $c_{I,s}$ in the solid phase , the adsorbed mass $\Delta M_{I,s}$ of substance I will be defined for pragmatic reasons in relation to the mass of the solid phase of the soil volume, since the corresponding phase volume at the surface area of the soil matrix usually is not well defined (Roth, 1996):

$$c_{I,s} = \frac{\Delta M_{I,s}}{\rho_s\ \Delta z^3} \quad , \tag{407}$$

where ρ_s $[kg\ m^{-3}]$ denotes the bulk density of the soil. Since the total mass ΔM_I of substance I can be expressed as the sum of mass in soil air $\Delta M_{I,a}$, of dissolved mass in soil water $\Delta M_{I,w}$ and the mass adsorbed to the solid phase $\Delta M_{I,s}$, the total concentration c_I is expressed as the sum of the fractions of concentrations in the different soil phases:

$$c_I = \eta\ c_{I,a}\ +\ \theta\ c_{I,w}\ +\ \rho_s\ c_{I,s} \tag{408}$$

If the substance dissolved in the soil water is always in direct equilibrium with the substance fraction adsorbed to the soil matrix, the adsorbed concentration $c_{I,s}$ $[kg\ kg^{-1}]$ of the substance I can be expressed by a function of the dissolved concentration $c_{I.w}$ $[kg\ m^{-3}]$, which is a linear function in the simplest case:

$$c_{I,s}\ =\ K_{I,d}\ c_{I,w} \tag{409}$$

This relationship is named the linear adsorption isotherm and the proportionality factor $K_{I,d}$ $[kg^{-1}\ m^3]$ is called adsorption coefficient.

In the same way, the concentration in the gaseous phase can be expressed as a function of the concentration in the liquid phase, if the concentrations in gaseous and liquid phase are in direct equilibrium. In the linear case, the following applies analogously

$$c_{I,a} \;=\; K_{I,H}\, c_{I,w} \quad , \tag{410}$$

where the proportionality factor $K_{I,H}$ is also called Henry constant .
In case of direct equilibrium between all three phases of the substance and linear relations between the substance concentrations, also the total concentration of the substance can be expressed as directly proportional to the substance concentration in the liquid phase:

$$c_I \;=\; (\eta\, K_{I,H} \;+\; \theta \;+\; \rho_s\, K_{I,d})\, c_{I,w} \tag{411}$$

In addition to the mass concentration we also consider the **flux concentration** $c^f_{I,w}$ of the soil solution, which is the ratio of solute mass flux and soil water flux:

$$c^f_{I,w} = \frac{q_{I,s}}{q_w} \quad , \tag{412}$$

where q_w $[m\ d^{-1}]$ denotes the water flux and $q_{I,s}$ $[kg\ m^{-2}\ d^{-1}]$ the solute mass flux within and with the soil water. The **solute mass flux** $q_{I,s}$ $[kg\ m^{-2}\ d^{-1}]$ gives the mass flux of the substance in soil solution, defined to be the mass of the substance I, which is transported dissolved in soil water per unit of time through a unit of cross-sectional area perpendicular to the direction of the water flux.

The flux concentration, which is obtained by averaging over a certain time step, is clearly different from the mass concentration, which is obtained by spatial averaging of the substance mass over a certain volume (Kreft and Zuber, 1978). Experimentally mass concentrations are often determined from soil samples, which are mainly taken by use of soil probes. Typically the concentrations obtained in this way describe vertical depth distributions of the substance or other spatial substance distributions at a specific time. In contrast, flux concentrations are often measured at the outlet of soil columns or lysimeters and usually describe breakthrough curves at certain depths of the soil profile (Roth, 1996).

In the following mass concentration will be only denoted concentration, while the designation flux concentration is maintained.

Substance source or sink terms, as they occur in the mass balance equations, will be denoted by $S_{c,I}$ for the substance I. They may be composed from terms Φ_I, which are obtained by single processes of substance turnover. Here we have to distinguish between amount of substance (e.g. often given in $[kg\ ha^{-1}]$) and concentration of substance (e.g. often given in $[mg\ dm^{-3}]$).

3.2.1.2 Law of mass conservation If mass fluxes within and with soil air are neglected, the following mass conservation law or **continuity equation** of vertical one-dimensional solute mass flux $q_{I,s}$ $[kg\ m^{-2}\ d^{-1}]$ of the substance I is given by the following relation:

$$\frac{\partial c_I}{\partial t} \;=\; -\,\frac{\partial q_{I,s}}{\partial z} \;+\; S_{c,I} \tag{413}$$

c_I	(mass-) concentration of substance I in the soil $[kg\ m^{-3}]$	t	time $[d]$
$S_{c,I}$	source or sink of substance I within the soil $[kg\ m^{-3}\ d^{-1}]$	z	depth $[m]$

3.2.1.3 Solute flux law of convection-dispersion Solute flux within and with the soil solution is composed by two fluxes, the flux by dispersion and the flux by convection.

The flux by dispersion describes the diffusion due to a concentration gradient within the soil solution and additionally the hydro-mechanical dispersion due to spatially different water flow paths within and through the pore space of the porous soil matrix. In analogy to the first of Fick's laws the **dispersive solute flux** can be expressed by a linear flux law:

$$q^d_{I,s} \;=\; -D_{I,e}\frac{\partial c_{I,w}}{\partial z} \tag{414}$$

$q^d_{I,s}$	dispersive solute flux $[kg\ m^{-2}\ d^{-1}]$	$D_{I,e}$	effective dispersion coefficient $[m^2\ d^{-1}]$
$c_{I,w}$	(mass-)concentration of the substance I in soil solution $[kg\ m^{-3}]$	z	depth $[m]$

The effective dispersion coefficient $D_{I,e}$ $[m^2\ d^{-1}]$ can be determined by the following relation (Bresler, 1973):

$$D_{I,e} \;=\; \theta\, f_\theta\, D_{I,o} \;+\; \lambda\,\sqrt{q_w^2} \quad , \tag{415}$$

$D_{I,o}$	molecular diffusion coefficient of substance I in the soil solution $[m^2\ d^{-1}]$		
θ	vol. water content $[1]$	f_θ	tortuosity factor $[1]$
λ	dispersivity $[m]$	q_w	vol. water flux $m\ d^{-1}$

where we assume, that the dispersivity λ is independent of water flow and depends only on soil depth z.

The **convective solute flux** is described by the following equation:

$$q^c_{I,s} \;=\; q_w\, c_{I,w} \tag{416}$$

$q^c_{I,s}$	convective solute mass flux $[kg\ m^{-2}\ d^{-1}]$
q_w	vol. water flux $[m\ d^{-1}]$
$c_{I,w}$	(mass-)concentration of substance I in soil solution $[kg\ m^{-3}]$

and hence it results the form of the **solute mass flux law of convection-dispersion**:

$$q_{I,s} = q^{d}_{I,s} \; + \; q^{c}_{I,s} \; = \; -D_e \, \frac{\partial c_{I,w}}{\partial z} \; + \; q_w \, c_{I,w} \tag{417}$$

$q^{d}_{I,s}$	diffusive solute mass flux $[kg\ m^{-2}\ d^{-1}]$	$q^{c}_{I,s}$	convective solute mass flux $[kg\ m^{-2}\ d^{-1}]$
$D_{I,e}$	effective dispersion coefficient $[m^2\ d^{-1}]$	q_w	vol. water flux $[m\ d^{-1}]$
$c_{I,w}$	(mass-)concentration of substance I in soil solution $[kg\ m^{-3}]$		

3.2.1.4 Transport Equation By insertion of the solute mass flux law (417) into the continuity equation (413) we obtain the following convection-dispersion transport equation:

$$\frac{\partial c_I}{\partial t} \; = \; \frac{\partial}{\partial z}\left[D_{I,e} \, \frac{\partial c_{I,w}}{\partial z} \; - \; q_w \, c_{I,w}\right] \; + \; S_{c,I} \tag{418}$$

c_I	total (mass-)concentration of substance I in soil $[kg\ m^{-3}]$
$c_{I,w}$	(mass-)concentration of substance I in soil solution $[kg\ m^{-3}]$
$D_{I,e}$	effective dispersion coefficient $[m^2\ d^{-1}]$
q_w	vol. water flux $[m\ d^{-1}]$
$S_{c,I}$	source or sink of substance I in soil $kg\ m^{-3}$

Under the assumption of equilibrium and linearity, which leads to the linear equation (411), results the linear partial parabolic differential equation in the unknown $c_{I,w}$, i.e. the linear convection-dispersion equation (CDE: convection-dispersion equation).

By neglecting the fraction of substance in the gaseous phase and considering the continuity equation of soil water flow (100), the linear transport equation can be further transformed and simplified, i.e. from equation

$$\frac{\partial \left[(\theta + \rho_s K_d) \; c_{I,w}\right]}{\partial t} \; = \; \frac{\partial}{\partial z}\left[D_{I,e} \, \frac{\partial c_{I,w}}{\partial z} \; - \; q_w \, c_{I,w}\right] \; + \; S_{c,I} \tag{419}$$

follows by differentiation:

$$\frac{\partial \theta}{\partial t} \, c_{I,w} + (\theta + \rho_s K_d) \, \frac{\partial c_{I,w}}{\partial t} \; = \; \frac{\partial}{\partial z}\left[D_{I,e} \, \frac{\partial c_{I,w}}{\partial z}\right] - \frac{\partial q_w}{\partial z} \, c_{I,w} - q_w \, \frac{\partial c_{I,w}}{\partial z} + S_{c,I} \tag{420}$$

and by insertion of the continuity equation of soil water flow (100):

$$(\theta + \rho_s K_d) \, \frac{\partial c_{I,w}}{\partial t} \; = \; \frac{\partial}{\partial z}\left[D_{I,e} \, \frac{\partial c_{I,w}}{\partial z}\right] \; - \; q_w \, \frac{\partial c_{I,w}}{\partial z} \; + \; S_{c,I} + S_w \, c_{I,w} \quad , \tag{421}$$

where S_w $[d^{-1}]$ denotes the sink of soil water within the considered soil volume.

3.2.2 Solute transport: Approach of the Model LEACHN

3.2.2.1 Transport equation Neglecting the air phase and assuming, that the phase of the substance dissolved in soil water and the phase adsorbed to the soil matrix are always in direct equilibrium and linearly related, the following one-dimensional solute transport equation of the concentration $c = c_I(t,z)$ in soil solution $[mg\ dm^{-3}]$ at time t $[d]$ in soil depth z $[mm]$ of the substance I:

$$\frac{\partial}{\partial t}\,[\,(\theta+\rho_s K_d)\ c\,]\ =\frac{\partial}{\partial z}[\,\theta D(\theta,q_w)\,\frac{\partial c}{\partial z}\ -\ q_w\ c\,]\ +\ S_{c,I} \tag{422}$$

$\theta = \theta(t,z)$	volumetric soil water content $[mm^3\ mm^{-3}]$
$\rho_s = \rho_s(z)$	soil bulk density $[kg\ dm^{-3}]$
$D(\theta,q_w) = D_I(\theta,q_w)$	dispersion coefficient $[mm^2\ d^{-1}]$ of substance I
$q_w = q_w(t,z)$	vol. water flux $[mm\ d^{-1}]$
$S_{c,I} = S_{c_I}(t,z)$	sink term $[mg\ dm^{-3}\ d^{-1}]$ of substance I
$K_d = K_{d,I}(z)$	adsorption coefficient $[dm^3\ kg^{-1}]$ of substance I

where the dispersion coefficient $D(\theta,q_w)$ of substance I is given by the following relationship :

$$\theta\ D(\theta,q_w)\ =\ D_o\,\alpha_D\ \exp(\beta_D\theta)\ +\ \lambda\,\sqrt{q_w^2} \tag{423}$$

$D_o = D_{o,I}$	molecular diffusion coefficient of substance I in the liquid Phase $[mm^2\ d^{-1}]$
α_D, β_D	empirical constants [1] according to Bresler (1973)
λ	dispersivity $[mm]$, see also Bresler (1973)

3.2.2.2 Initial and Boundary conditions As initial condition at simulation start at time t_0 $[s]$ a depth distribution of the concentration $c_0 = c_0(z)$ of substance I has to be given as a function of depth z for the total considered soil profile:

$$c_I(t,z) = c_0(z) \quad \text{for} \quad t = t_0 \tag{424}$$

An upper boundary condition for the solute mass flux q_s $[g\ m^{-3}\ d^{-1}]$ across the soil surface is prescribed by:

$$q_s = \begin{cases} q_w\ c_s & \text{for}\ \ q_w > 0\ \ \text{(infiltration)} \\ 0 & \text{for}\ \ q_w \leq 0\ \ \text{(evaporation)} \end{cases} \tag{425}$$

c_s	solute concentration in infiltration water $[g\ m^{-3}]$	q_w	water flux of infiltration $[mm\ d^{-1}]$

As lower boundary condition at depth ℓ a solute concentration c_ℓ is prescribed:

$$c_I(t,\ell) = c_\ell \tag{426}$$

where c_ℓ is given depending on water flow: $c_\ell = c_0(\ell)$ at free drainage, $c_\ell = 0$ at no drainage and $c_\ell = c_g$ at saturated conditions in depth ℓ in connection with groundwater, in which the substance I occurs with solute concentration c_g.

3.2.2.3 Numerical Solution The transport equation together with the corresponding initial and boundary conditions is numerically solved by a finite difference method . The related discretisation of the transport equation folllows Bresler (1973), neglecting terms of second order (Tillotson et al., 1980). The difference expression of the first term of the left hand side of equation (425) at spatial knot i for the time interval from j to j+1 results from:

$$\left(\frac{\partial(\theta c)}{\partial t}\right)_i^{j+\frac{1}{2}} = \frac{\theta_i^{j+1}c_i^{j+1} - \theta_i^j c_i^j}{\Delta t^{j+1}} \tag{427}$$

θ_i^{j+1}	volumetric water content of the i-th soil layer at time step j+1
θ_i^j	volumetric water content of the i-th soil layer at time step j
c_i^{j+1}	substance concentration in soil solution of the i-th soil layer at time step j+1
c_i^j	substance concentration in soil solution of the i-th soil layer at time step j
Δt^{j+1}	time step difference $t^{j+1} - t^j$

accordingly results the second term from

$$\left(\rho_s K_d \frac{\partial c}{\partial t}\right)_i^{j+\frac{1}{2}} = \rho_{s,i} K_{d,i} \frac{c_i^{j+1} - c_i^j}{\Delta t^{j+1}} \tag{428}$$

$\rho_{s,i}$	bulk density of the i-th soil layer
$K_{d,i}$	Adsorption coefficient of the i-th soil layer
c_i^{j+1}	substance conzentration in soil solution of the i-th soil layer at time step j+1
c_i^j	substance concentration in soil solution of the i-th soil layer at time step j
Δt^{j+1}	time step difference $t^{j+1} - t^j$

The dispersion coefficient $D_{i+1/2}^{j+1/2}$ of the i-th soil layer between the knots i and i+1 and of the time interval between j and j+1 is discretised by the following expression:

$$\theta_{i+\frac{1}{2}}^{j+\frac{1}{2}} D_{i+\frac{1}{2}}^{j+\frac{1}{2}} = \lambda\sqrt{(q_{i+\frac{1}{2}}^{j+\frac{1}{2}})^2} + D_o \alpha_D \exp(\beta_D \theta_{i+\frac{1}{2}}^{j+\frac{1}{2}}) \tag{429}$$

$$\theta_{i+\frac{1}{2}}^{j+\frac{1}{2}} = (\theta_{i+1}^{j+1} + \theta_{i+1}^{j} + \theta_{i}^{j+1} + \theta_{i}^{j})/4$$

$$q_{i+\frac{1}{2}}^{j+\frac{1}{2}} = -K_{i+\frac{1}{2}}^{j} (h_{i+1}^{j+1} + h_{i}^{j+1} + h_{i+1}^{j} + h_{i}^{j} - 2\Delta z)/(2\Delta z)$$

Expression (429) is further corrected for numerical dispersion according to (Hutson und Wagenet 1992).

For the first term of the right hand side of equation (422) one gets

$$(\frac{\partial}{\partial z}[\theta D(\theta, q_w)\frac{\partial c}{\partial z}]\,)_i^{j+\frac{1}{2}} \;=\; \tag{430}$$

$$\frac{1}{2(\Delta z)^2}\,[\, D_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,\theta_{i+\frac{1}{2}}^{j+\frac{1}{2}}\,(c_{i+1}^{j+1} - c_i^{j+1} + c_{i+1}^{j} - c_i^{j}) \;-\; D_{i-\frac{1}{2}}^{j+\frac{1}{2}}\,\theta_{i-\frac{1}{2}}^{j+\frac{1}{2}}\,(c_i^{j+1} - c_{i-1}^{j+1} + c_i^{j} + c_{i-1}^{j})\,]$$

The second term of the right hand side, the convection term is discretized depending on the direction of the actual water flux between the (i-1)-, i-, and (i+1)-th soil layer:

$$\frac{\partial}{\partial z}\,(\,q_w\;c\,)_i^{j+\frac{1}{2}} \;=\; \tag{431}$$

$$\begin{aligned}
&\beta_1\;q_{i-\frac{1}{2}}^{j+\frac{1}{2}}\;(\,c_{i-1}^{j+1}\;+\;c_{i-1}^{j}\,)/(2\Delta z)\\
&-\beta_2\;q_{i+\frac{1}{2}}^{j+\frac{1}{2}}\;(\,c_i^{j+1}\;+\;c_i^{j}\,)/(2\Delta z)\\
&-\beta_3\;q_{i+\frac{1}{2}}^{j+\frac{1}{2}}\;(\,c_{i+1}^{j+1}\;+\;c_{i+1}^{j}\,)/(2\Delta z)\\
&+\beta_4\;q_{i-\frac{1}{2}}^{j+\frac{1}{2}}\;(\,c_i^{j+1}\;+\;c_i^{j}\,)/(2\Delta z)
\end{aligned}$$

where

$$\begin{aligned}
\beta_1 &= 1\ and\ \beta_4 = 0\ if\ q_{i-\frac{1}{2}}^{j+\frac{1}{2}} > 0\,,\\
\beta_1 &= 0\ and\ \beta_4 = 1\ if\ q_{i-\frac{1}{2}}^{j+\frac{1}{2}} < 0\,,\\
\beta_2 &= 1\ and\ \beta_3 = 0\ if\ q_{i+\frac{1}{2}}^{j+\frac{1}{2}} > 0\,,\\
\beta_2 &= 0\ and\ \beta_3 = 1\ if\ q_{i+\frac{1}{2}}^{j+\frac{1}{2}} < 0\,.
\end{aligned}$$

q_w	vol. water flux $[mm\ d^{-1}]$
c	substance concentration in soil solution $[g\ m^{-3}]$
β_i	coefficients of adaptation to water flow direction [1]
Δz	thickness of soil layer $[mm]$

If one replaces in equation (422) the single terms by the corresponding difference expressions and adds the sink term, a tridiagonal linear equation system results, which then is solved by the elimination method of Gauss (cf. 1.4.4.5) again.
Three nitrogen species, urea $(NH_2)_2CO$, ammonium NH_4^+, and nitrate NO_3^-, are considered by the model LEACHN to simulate their transport in and with the soil water.
For each of the three nitrogen species a transport equation in the form of equation (422) is used and completed by corresponding sink terms $S_{c,I}$ ($I = UR$ in case of urea, $I = NH$ incase of ammonium, and $I = NO$ in case of nitrate). In case of N-transformation the three resulting transport equations are then coupled by the sink terms.

3.2.3 Nitrate transport: Approach of the model CERES-N

The model CERES-N only considers the transport of nitrate. In case of ammonium it is assumed, that no transport occurs between soil layers. Nitrate transport or nitrate leaching is modeled per time step depending on soil water flow. For the i-th soil layer the calculated actual volumetric soil water content and the simulated percolating amount of water Q_i per time step between the i-th and (i+1)-th soil layer are used to determine the nitrate leaching from this soil layer:

$$N^t_{out,i} = N^t_{NO,i} \quad \frac{Q_i}{\theta_i d_i + Q_i} \tag{432}$$

t	actual time $[d]$
$N^t_{out,i}$	amount of nitrate-N $[kg\ ha^{-1}]$ leached from the i-th soil layer
$N^t_{NO,i}$	Nitrate amount in the i-th soil layer $[kg\ ha^{-1}]$
Q_i	amount of water percolating from the i-th to the (i+1)-th soil layer $[mm]$
θ^t_i	vol. water content $[mm^3\ mm^{-3}]$ of the i-th soil layer at time t
d_i	layer thickness $[mm]$ of the i-th soil layer

Each percolation event therefore leads to the transport of a part of the nitrate amount stored in the respective soil layer. Following this simple capacity or cascade approach, the loss of nitrate from this layer is then added to the nitrate amount of the underlying soil layer. In case the nitrate-N concentration of a soil layer falls below 0,5 mg NO_3-N/kg soil, no further nitrate leaching from this layer is simulated.

For this approach it is assumed, that the total nitrate is homogeneously and completely dissolved in the total soil water of the respective soil layer. It is not considered to partition the nitrate to mobile and immobile water. Differences of transport behaviour between soils of different textures , are considered as function of the relative size of volumetric water content at field capacity θ_{fc} and water saturation θ_{max}. Compared to a clay soil, in a sandy soil nitrate is more strongly leached, since the ratio of the potential percolating water amount $(\theta_{max} - \theta_{fc})\ d_i$ to the water amount stored at field capacity $\theta_{fc}\ d_i$ is considerably higher than in case of heavy soils.

3.2.4 Nitrous oxide transport: Approach of the Model EXPERT-N

The Model EXPERT-N can also be applied to simulate the one- dimensional vertical transport of nitrous oxide (N_2O) in the soil profile by a convection-dispersion equation. For this purpose it is assumed, that there is a direct equilibrium between the N_2O in soil air and the N_2O dissolved in the soil solution and that the N_2O-concentration in the gas phase is directly proportional to the N_2O-concentration in the liquid phase:

$$\frac{\partial}{\partial t}\,[(\theta_{sat}-\theta+\theta\,K_H^{-1})\,c_{N_2O}] \;=\; \frac{\partial}{\partial z}[D(\theta,q_w)\,\frac{\partial c_{N_2O}}{\partial z} - q_w\,K_H^{-1}\,c_{N_2O}] \,+\, S_{c,N_2O} \quad (433)$$

$$S_{c,N_2O} = k_{nit,N_2O} \,+\, k_{den,N_2O} \,-\, k_{red,N_2} \quad (434)$$

θ	volumetric water content $[mm^3\ mm^{-3}]$
θ_{sat}	saturated vol. water content $[mm^3\ mm^{-3}]$
$K_H = K_{N_2O,H}$	Henry constant [1], the distribution coefficient or proportionality factor between the N_2O-concentrations in gaseous and liquid phase
$D(\theta,q_w)$	diffusions-dispersion coefficient $[mm^2\ d^{-1}]$
q_w	vol. water flux $[mm\ d^{-1}]$
c_{N_2O}	gaseous N_2O-concentration $[mg\ dm^{-3}]$ in soil air
k_{Nit,N_2O}	N_2O production rate during nitrification $[mg\ dm^{-3}\ d^{-1}]$
k_{den,N_2O}	N_2O production rate during denitrification $[mg\ dm^{-3}\ d^{-1}]$
k_{red,N_2}	reduction rate of N_2O to N_2 $[mg\ dm^{-3}\ d^{-1}]$

The diffusion-dispersion coefficient $D(\theta,q_w)$ here is given by

$$D(\theta,q_w) \;=\; D_{og}\,\frac{(\theta_{sat}-\theta)^{10/3}}{\theta_{sat}^2} \,+\, \theta\,K_H^{-1}[D_{ol}\,\beta_D\exp(\alpha_D\theta)+\lambda\sqrt{q_w^2}], \quad (435)$$

where the first term denotes the effective gas diffusion coefficient, which presents the product of the molecular diffusion coefficient D_{og} $[mm^2\ d^{-1}]$ of N_2O in the gaseous phase and the Millington-Quirk tortuosity factor (Jin and Jury, 1996).

The second factor of the second term is the diffusion-dispersion coefficient of N_2O related to the liquid phase. It is given by the sum of the effective diffusion coefficient in soil solution and the hydro-mechanical dispersion coefficient. The effective diffusion coefficient is given by the product of the diffusion coefficient of N_2O in soil solution D_{ol} $[mm^2\ d^{-1}]$ and the soil solution tortuosity factor $\beta_D\exp(\alpha_D\theta)$ [1] with fixed parameters α_D and β_D according to Bresler (1973), see equation (423). The mechanical dispersion coefficient is calculated from the dispersivity λ $[mm]$ and the vol. water flux q_w $[mm\ d^{-1}]$ according to Bresler (1973).

The N_2O-transport model is completed by the equations, which define the boundary conditions. For the upper boundary it is assumed, that the exchange of N_2O in gaseous form between soil air at the soil surface and the air above the soil is determined by the vertical gradient of the gaseous N_2O-concentration at the soil surface. It is further assumed, that this gradient is directly proportional to the difference between the N_2O-soil air concentration in the upper most soil directly at the soil surface $c_{N_2O,top}$ $[mg\ dm^{-3}]$ and the average N_2O-concentration in the atmosphere $c_{N_2O,atm}$ $[mg\ dm^{-3}]$ near the soil surface, where κ $[mm^{-1}]$ represents the proportionality factor:

$$\left.\frac{\partial c_{N_2O}}{\partial z}\right|_{z=0} = \kappa\,(c_{N_2O,top} - c_{N_2O,atm}) \tag{436}$$

At the lower end of the soil profile, at depth ℓ, it is assumed, that the vertical N_2O-concentration gradient hardly changes any more:

$$\left.\frac{\partial c_{N_2O}}{\partial z}\right|_{z=\ell} = 0 \tag{437}$$

Finally, the mass transport equation for N_2O is solved according to the same numerical procedure used in the model LEACHN for the soil solute transport equation.

3.2.5 Two-region solute transport equation: Approach of the model WAVE

The solute transport equation, which is used by the model WAVE (Vanclooster et al., 1994) extends the classical one-dimensional vertical convection-dispersions equation given by Bresler (1973) to a two-region solute transport model according to van Genuchten and Wierenga (1976). The implementation and numerical solution of this model into EXPERT-N however does not follow the discretisation of Bresler (1973) and Tillotson et al. (1980) as also used by the modell WAVE, but directly follows the way of discretisation applied by the model LEACHN.

3.2.5.1 Transport equations For the two-region transport model the water filled pore volume of the soil is partitioned into two regions, the pore region of mobile water and the pore region of immobile water. In addition, a distinction is made between sorption sites of the solid soil matrix, that are in contact with the soil solution of the mobile water or that of the immobile water. The resulting transport equations, which determine the solute flux in and with the soil solution and the exchange between mobile and immobile region (van Genuchten and Wierenga, 1976) are then given by:

$$\frac{\partial}{\partial t}\left[\,(\theta_m + f\rho_s K_d)\,c_m\,\right] = \frac{\partial}{\partial z}\left[\,\theta_m D_I(\theta_m, q_w)\,\frac{\partial c_m}{\partial z} - q_w\,c_m\,\right] - \alpha\,(c_m - c_{im}) + S_{c,I,m} \tag{438}$$

$$\frac{\partial}{\partial t}\left[\,(\theta_{im} + (1-f)\rho_s K_d)\,c_{im}\,\right] = \alpha\,(c_m - c_{im}) + S_{c,I,im} \tag{439}$$

$\theta_m = \theta_m(t,z)$	mobile volumetric water content $[mm^3\ mm^{-3}]$
$\theta_{im} = \theta_{im}(t,z)$	immobile volumetric water content $[mm^3\ mm^{-3}]$
$f = f(z)$	fraction of sorption sites within the mobile region [1]
$\rho_s = \rho_s(z)$	soil bulk density $[kg\ dm^{-3}]$
$c_m = c_m(t,z)$	solute concentration in the mobile soil solution $[mg\ dm^{-3}]$
$c_{im} = c_{im}(t,z)$	solute concentration in the immobile soil solution $[mg\ dm^{-3}]$
$D_I(\theta_m, q_w)$	dispersion coefficient $[mm^2\ d^{-1}]$ of substance I
$q_w = q_w(t,z)$	vol. water flux $[mm\ d^{-1}]$
$S_{c,I,m}$	sink term $[mg\ dm^{-3}\ d^{-1}]$ of the mobile fraction
$S_{c,I,im}$	sink term $[mg\ dm^{-3}\ d^{-1}]$ of the immobile fraction
$K_d = K_{d,I}(z)$	equilibrium-adsorption constant $[dm^3\ kg^{-1}]$
$\alpha = \alpha(z) > 0$	solute transfer coefficient $[d^{-1}]$ between mobile and immobile region

where the term $Q = \alpha(c_m - c_{im})$ describes the solute exchange respectively the delayed convergence of solute concentrations between the two regions.

3.2.5.2 Boundary Conditions The boundary conditions of the transport equation (438) are given by a flux boundary condition at the upper boundary and by a von Neumann condition (Schwarz, 1986) at the lower boundary:

As upper boundary condition we have for the solute flux across the soil surface q_s $[g\ m^{-3}\ d^{-1}]$:

$$q_s = \begin{cases} q_w\ c_s & \text{for} \quad q_w > 0 \quad \text{(infiltration)} \\ 0 & \text{for} \quad q_w \leq 0 \quad \text{(evaporation)} \end{cases} \tag{440}$$

c_s solute concentration within infiltration water $[g\ m^{-3}]$ q_w water flux of infiltration $[mm\ d^{-1}]$

As lower boundary condition a homogeneous distribution of solute concentration is assumed to be present at the lower end of the soil profile at ℓ $[mm]$, i.e. we assume an almost zero concentration gradient at depth ℓ:

$$\left. \frac{\partial c_m}{\partial z} \right|_{x=\ell} = 0 \tag{441}$$

3.2.5.3 Numerical Solution From the discretisation of equation (438) analogously to the finite difference discretisation of the transport equation used by the model LEACHN follows the tridiagonal equation system corresponding to the spatial steps ($2 \leq i \leq n-1$) and the time steps ($1 \leq j \leq m$):

$$A_i\, c_{m,i-1}^{j+1} + B_i\, c_{m,i}^{j+1} + C_i\, c_{m,i+1}^{j+1} = D_i \tag{442}$$

with coefficients:

$$\begin{aligned} A_i &= -AB_i - \beta_1\, CB_i & (443) \\ B_i &= (\theta_{m,i}^{j+1} + f_i\, \rho_{s,i}\, K_{d,i})/\Delta t + AB_i + BB_i + \beta_2\, DB_i - \beta_4\, CB_i & (444) \\ C_i &= -\, BB_i + \beta_3\, DB_i & (445) \\ D_i &= c_{m,i-1}^{j}\, (AB_i + \beta_1 CB_i) \\ &\quad + c_{m,i}^{j}\, [(\theta_{m,i}^{j} + f_i\, \rho_{s,i}\, K_{d,i})/\Delta t - AB_i - BB_i - \beta_2\, DB_i + \beta_4\, CB_i] \\ &\quad + c_{m,i+1}^{j}\, (BB_i - \beta_3 DB_i) \\ &\quad + S_{c,I,m,i} - \alpha_i (c_{m,i}^{j} - c_{im,i}^{j}) & (446) \end{aligned}$$

using abbreviations:

$$\begin{aligned} AB_i &= \theta_{m,i-\frac{1}{2}}^{j+\frac{1}{2}}\, D_{I,i-\frac{1}{2}}^{j+\frac{1}{2}}/(2\Delta z^2) & (447) \\ BB_i &= \theta_{m,i+\frac{1}{2}}^{j+\frac{1}{2}}\, D_{I,i+\frac{1}{2}}^{j+\frac{1}{2}}/(2\Delta z^2) & (448) \\ CB_i &= q_{i-\frac{1}{2}}^{j+\frac{1}{2}}/(2\Delta z) & (449) \\ DB_i &= q_{i+\frac{1}{2}}^{j+\frac{1}{2}}/(2\Delta z) & (450) \end{aligned}$$

The upper and lower boundary conditions lead to the equations for $(i = 1)$ and $(i = n)$, which complete the tridiagonlal equation system:
For the upper boundary we have $(i = 1)$:

$$B_1\, c_{m,1}^{j+1} \;+\; C_1\, c_{m,2}^{j+1} \;=\; D_1 \tag{451}$$

with coefficients

$$\begin{aligned}
B_1 &= (\theta_{m,1}^{j+1} + f_1\, \rho_{s,1}\, K_{d,1})/\Delta t + \beta_2\, DB_1 - \beta_4\, CB_1 && (452)\\
C_1 &= \beta_3\, DB_1 && (453)\\
D_1 &= (c_s^j \;-\; c_s^{j+1})\; \beta_1 CB_1 \\
&\quad + c_{m,1}^j\, [(\theta_{m,1}^j + f_1\, \rho_{s,1}\, K_{d,1})/\Delta t - \beta_2\, DB_1 + \beta_4\, CB_1] \\
&\quad + c_{m,2}^j\, (-\beta_3 DB_i) \\
&\quad + S_{c,I,m,1} \;- \alpha_1(c_{m,1}^j - c_{im,1}^j) && (454)
\end{aligned}$$

and abbreviations:

$$\begin{aligned}
CB_1 &= q_{1-\frac{1}{2}}^{j+\frac{1}{2}}/(2\Delta z) && (455)\\
DB_1 &= q_{1+\frac{1}{2}}^{j+\frac{1}{2}}/(2\Delta z) && (456)
\end{aligned}$$

For the lower boundary $(i = n)$ follows $c_{m,n}^{j+1} = c_{m,n+1}^{j+1}$, i.e.:

$$A_n\, c_{m,n-1}^{j+1} \;+\; B_n\, c_{m,n}^{j+1} \;=\; D_n \tag{457}$$

with coefficients

$$\begin{aligned}
A_n &= -AB_n \;-\; \beta_1\, CB_n && (458)\\
B_n &= (\theta_{m,n}^{j+1} + f_n\, \rho_{s,n}\, K_{d,n})/\Delta t + AB_n + \beta_2\, DB_n + \; \beta_3\, DB_i - \beta_4\, CB_n && (459)\\
D_n &= c_{m,n-1}^j\, (AB_n + \beta_1 CB_n) \\
&\quad + c_{m,n}^j\, [(\theta_{m,n}^j + f_n\, \rho_{s,n}\, K_{d,n})/\Delta t - AB_n - \beta_2\, DB_n - \beta_3 DB_i + \beta_4\, CB_n] \\
&\quad + S_{c,I,m,n} \;- \alpha_n(c_{m,n}^j - c_{im,n}^j) && (460)
\end{aligned}$$

and abbreviations:

$$\begin{aligned}
AB_n &= \theta_{m,n-\frac{1}{2}}^{j+\frac{1}{2}}\; D_{I,n-\frac{1}{2}}^{j+\frac{1}{2}}/(2\Delta z^2) && (461)\\
CB_n &= q_{n-\frac{1}{2}}^{j+\frac{1}{2}}/(2\Delta z) && (462)\\
DB_n &= q_{n+\frac{1}{2}}^{j+\frac{1}{2}}/(2\Delta z) && (463)
\end{aligned}$$

The Taylor expansion of the term of the left hand side of the mass balance equation (439) for the immobile region leads to the following expressions by applying the abbreviation $g_i^j = \theta_{im,i}^j + (1-f_i)\rho_i K_{d,i}$ for $(1 \leq i \leq n)$ (Vanclooster et al., 1994) for negative α:

$$\frac{\partial(g_i\ c_{im,i})}{\partial t} = \frac{g_i^{j+1}\ c_{im,i}^{j+1} - g_i^j\ c_{im,i}^j}{\Delta t} + \frac{\Delta t}{2}\ \frac{\partial^2(g_i\ c_{im,i})}{\partial t^2} \tag{464}$$

The final expansion of the term of second order leads to:

$$\begin{aligned}\frac{\partial^2(g_i\ c_{im,i})}{\partial t^2} &= \frac{\partial}{\partial t}[\alpha_i\ (c_{m,i} - c_{im,i}) + S_{c,I,im,i}] \\ &= \frac{\alpha_i\ (c_{m,i}^{j+1} - c_{m,i}^j)}{\Delta t} - \frac{\alpha_i\ (c_{im,i}^{j+1} - c_{im,i}^j)}{\Delta t} + \frac{S_{c,I,im,i}^{j+1} - S_{c,I,im,i}^j}{\Delta t}\end{aligned} \tag{465}$$

By insertion of this equation and transformation results the discretization of the mass balance equation (439):

$$E_i\ c_{im,i}^{j+1} = F_i\ c_{im,i}^j - \tfrac{1}{2}\,\alpha_i(c_{m,i}^{j+1} - 3\ c_{m,i}^j) + \tfrac{1}{2}\,(S_{c,I,im,i}^{j+1} - S_{c,I,im,i}^j) \tag{466}$$

with the abbreviations:

$$E_i = \frac{\theta_{im,i}^{j+1} + (1-f_i)\rho_{s,i}K_{d,i}}{\Delta t} - \frac{1}{2}\,\alpha_i \tag{467}$$

$$F_i = \frac{\theta_{im,i}^{j} + (1-f_i)\rho_{s,i}K_{d,i}}{\Delta t} - \frac{3}{2}\,\alpha_i \tag{468}$$

3.2.6 Solute transport: Approach of the model HYDRUS

The numerical method applied by the model HYDRUS (van Genuchten, 1982; Vogel et al., 1996; Simunek et al., 1998) to solve the nonlinear solute transport equation is similar to the approach used by HYDRUS to solve the water flow equation or Richards equation and is based again on a finite-element-method (FEM) of discretisation.

3.2.6.1 Transport Equation Starting point is the classical convection-dispersion equation:

$$\frac{\partial(\theta c_w)}{\partial t} + \frac{\partial(\rho_s c_s)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c_w}{\partial z}\right) - \frac{\partial(q_w c_w)}{\partial z} + S_c \tag{469}$$

θ	volumetric water content $[mm^3\ mm^{-3}]$
c_w	concentration in soil solution $[mg\ dm^{-3}]$
ρ_s	bulk density of soil $[kg\ dm^{-3}]$
c_s	adsorbed concentration at the solid phase $[mg\ dm^{-3}]$
$D = D(\theta, q_w)$	dispersion coefficient $[mm^2\ d^{-1}]$
$q_w = q_w(t, z)$	vol. water flux $[mm\ d^{-1}]$
S_c	source- resp. sink term $[mg\ dm^{-3}\ d^{-1}]$

The dispersion coefficient D $[mm^2\ d^{-1}]$ is given by the molecular diffusion coefficient D_o $[mm^2\ d^{-1}]$ in water, by a tortuosity factor τ [1] and the dispersivity λ $[mm^2\ d^{-1}]$:

$$D = D_o \tau + \lambda \frac{\sqrt{q_w^2}}{\theta}, \tag{470}$$

where the tortuosity factor τ is calculated by the relation according to Millington and Quirk (1961):

$$\tau = \frac{\theta^{7/3}}{\theta_{sat}^2} \tag{471}$$

θ	vol. water content $[mm^3\ mm^{-3}]$	θ_{sat}	saturated vol. water content $[mm^3\ mm^{-3}]$

For the description of adsorption in direct equilibrium with the soil solution it is assumed that a nonlinear Freundlich isotherm represents the relation between the adsorbed concentration and the soil solution concentration:

$$c_s = K_f\ c_w^{n_f} \tag{472}$$

In case the Freundlich isotherm exponent n_f [1] is equal to one: $n_f = 1$, the Freundlich isotherm is linear and the adsorption coefficient K_f $[g^{-1}\ dm^3]$ is then identical to the distribution coefficient K_d $[g^{-1}\ dm^3]$, i.e. equal to the linear adsorption coefficient (s. section 3.2.1.1).

By insertion of eq. (472) into eq. (469) and by definition of the retardation coefficient R [1]

$$R = 1 + \frac{\rho_s \, K_f \, c_w^{n_f - 1}}{\theta} \tag{473}$$

we get the form of the transport equation, which is finally numerically solved by the finite element method:

$$\frac{\partial(\theta R c_w)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c_w}{\partial z}\right) - \frac{\partial(q_w c_w)}{\partial z} + S_c \tag{474}$$

θ	vol. water content $[mm^3 \; mm^{-3}]$	R	retardation coefficient [1]
c_w	soil solution concentration $[mg \; dm^{-3}]$	D	dispersion coefficient $[mm^2 \; d^{-1}]$
q_w	vol. water flux $[mm \; d^{-1}]$	S_c	sink- resp. source term $[mg \; dm^{-3} \; d^{-1}]$

3.2.6.2 Initial- and Boundary Conditions

The transport equation is solved assuming the general initial condition

$$c_w(t,z) = c_\alpha(z) \quad \text{for} \quad t = t_0 \tag{475}$$

where c_α is a general function of the depth z and of the start time t_0 of the simulation.

As boundary condition at the upper end, i.e. at depth $z = 0$ of the soil profile, a Dirichlet condition can be prescribed:

$$c_w(t,z) = c_0(t) \quad \text{for} \quad z = 0 \quad , \tag{476}$$

where c_0 represents the soil solution concentration at the soil surface by a general function of time. Alternatively a flux boundary condition can be chosen:

$$(-\theta D \frac{\partial c}{\partial z})\Big|_{z=0} = \begin{cases} q_0 \; c_0(t) & \text{for } q_0 > 0 \\ 0 & \text{for } q_0 \leq 0 \end{cases} \quad , \tag{477}$$

where c_0 represents the solute concentration in the infiltration water as general function of time and q_0 denotes the volumetric water flux across the soil surface. Here, the water flux is positive, if directed downwards (to the center of Earth) and negative in case of upward flux (s. section 1.4.1 Notation).

At the lower end of the soil column at depth $z = \ell$ a zero gradient boundary condition is useful, if drainage, i.e. the case $q_w(t,\ell) > 0$, is considered:

$$\frac{\partial c}{\partial z} = 0 \quad \text{for} \quad z = \ell \tag{478}$$

In the case of upward flow conditions out of the ground water, $q_w(t,\ell) < 0$, if $z = \ell$ represents also the height of the groundwater level, a Dirichlet condition can be applied:

$$c_w(t,z) = c_\ell(t) \quad \text{for} \quad z = \ell \quad , \tag{479}$$

where c_ℓ represents the solute concentration of groundwater at depth $z = \ell$ as a function of time.

3.2.6.3 Numerical Solution The solute transport equation (474) is solved similarly to the numerical solution of the Richards equation of the HYDRUS model (s. section 1.4.5.1) by use of the finite element method of Galerkin. The piece-wise linear approximation of the soil solution concentration $\widetilde{c_w}(t,z)$ is then given by:

$$\widetilde{c_w}(t,z) = \sum_{i=1}^{n+1} \widetilde{c}_i(t)\phi_i(z) \tag{480}$$

For this, the functions $\widetilde{c}_i$ are defined by $\widetilde{c}_i(t) := \widetilde{c_w}(t, z_i)$ and the basis functions ϕ_i are given by splitting the interval $[0,\ell]$ into n sub-intervals $[z_i, z_{i+1}]$. The orthogonality condition for the basis functions leads to

$$\int_0^\ell \left[\frac{\partial(\theta R\widetilde{c_w})}{\partial t} - \frac{\partial}{\partial z}\left(\theta D \frac{\partial \widetilde{c_w}}{\partial z}\right) + \frac{\partial(q_w \widetilde{c_w})}{\partial z} - \Phi \right] \phi_i dz = 0 \quad , \tag{481}$$

for all $1 \le i \le n+1$, and partial integration of the spatial derivations leads to

$$\int_0^\ell \frac{\partial(\theta R\widetilde{c_w})}{\partial t}\, \phi_i dz - \int_0^\ell Q_s\, \frac{\partial \phi_i}{\partial z} dz - \int_0^\ell \Phi\ \phi_i dz = -Q_s\phi_i \Big|_0^\ell \quad , \tag{482}$$

for all $1 \le i \le n+1$, where the following abbreviation was used:

$$Q_s = -\theta D \frac{\partial \widetilde{c_w}}{\partial z} + q_w \widetilde{c_w} \tag{483}$$

Similar as in section 1.4.5.1 by insertion of the sum expression for the approximating function $\widetilde{c_w}$ and related 'mass lumping' of the capacity term, i.e. the first term of equation (482), we get the following systems of equations:

$$\mathbf{B}\, \frac{d\widetilde{\mathbf{c}}}{dt} \ +\ \mathbf{A}\, \widetilde{\mathbf{c}} \ =\ \mathbf{f} \tag{484}$$

for the vectors $\widetilde{\mathbf{c}}$ and **f**, and the matrices **A** and **B**, for which we have

$$A_{ij} \ = \ A^q_{ij} + A^D_{ij} \ = \sum_e \int_{\Omega_e} -\left(q_w\phi_j - \theta D \frac{d\phi_j}{dz}\right) \frac{d\phi_i}{dz}\, dz \tag{485}$$

$$\begin{aligned} A^q_{ij} \ &= \ \sum_e \int_{\Omega_e} -q_w \phi_j \frac{d\phi_i}{dz}\, dz = \sum_{e=i}^{i+1} \int_{\Omega_e} \sum_{k=e-1}^{e} -q_k\phi_k\ \phi_j \frac{d\phi_i}{dz}\, dz = \\ &= \begin{cases} -(2q_{i-1} + q_i)/6 & \text{for } i-1 = j \\ (q_{i+1} - q_{i-1})/6 & \text{for } i = j \\ (q_i + 2q_{i+1})/6 & \text{for } i+1 = j \\ \qquad 0 & \text{for } |i-k| > 1 \end{cases} \end{aligned} \tag{486}$$

$$\begin{aligned} A_{ij}^{D} &= \sum_e \int_{\Omega_e} \theta D \frac{d\phi_j}{dz}\frac{d\phi_i}{dz}\,dz = \sum_{e=i}^{i+1} \int_{\Omega_e} \sum_{k=e-1}^{e} \theta_k D_k \phi_k \frac{d\phi_j}{dz}\frac{d\phi_i}{dz}\,dz = \\ &= \begin{cases} -(\theta_{i-1}D_{i-1} + \theta_i D_i)/(2\Delta z) & \text{for } i-1=j \\ (\theta_{i-1}D_{i-1} + 2\,\theta_i D_i + \theta_{i+1}D_{i+1})/(2\Delta z) & \text{for } i=j \\ -(\theta_i D_i + \theta_{i+1}D_{i+1})/(2\Delta z) & \text{for } i+1=j \\ \qquad 0 & \text{for } |i-k|>1 \end{cases} \end{aligned} \tag{487}$$

$$\begin{aligned} B_{ij} &= \sum_e \int_{\Omega_e} \theta R \phi_j\ \phi_i\,dz = \sum_{e=i}^{i+1} \int_{\Omega_e} \sum_{k=e-1}^{e} \theta_k R_k \phi_k \phi_j\ \phi_i\,dz = \\ &= \begin{cases} (\theta_{i-1}R_{i-1} + \theta_i R_i)\ \Delta z/12 & \text{for } i-1=j \\ (\theta_{i-1}R_{i-1} + 6\,\theta_i R_i + \theta_{i+1}R_{i+1})\ \Delta z/12 & \text{for } i=j \\ (\theta_i R_i + \theta_{i+1}R_{i+1})\ \Delta z/12 & \text{for } i+1=j \\ \qquad 0 & \text{for } |i-k|>1 \end{cases} \end{aligned} \tag{488}$$

$$\frac{d\widetilde{c}_i}{dt} := \left(\int_\Omega \theta R\,\frac{\partial \widetilde{c}}{\partial t}\,\phi_i\,dz\right)/\left(\int_\Omega \theta R \phi_i\,dz\right) \qquad \text{'mass lumping'} \tag{489}$$

$$\begin{aligned} f_i &= \sum_e \int_{\Omega_e} S_c \phi_i\,dz - Q_s \phi_i \Big|_0^\ell = \\ &= \sum_{e=i}^{i+1} \int_{\Omega_e} \sum_{k=e-1}^{e} S_{c,k}\phi_k\phi_i\,dz - q_s(t,\ell)\phi_i(\ell) + q_s(t,0)\phi_i(0) = \\ &= (S_{c,i-1} + 4\,S_{c,i} + S_{c,i+1})\ \Delta z/6 - q_s(t,\ell)\phi_i(\ell) + q_s(t,0)\phi_i(0) \end{aligned} \tag{490}$$

for all $1 < i < n+1$.

The corresponding equations of the boundary conditions are completing the spatial discretisation of the solute transport equation. The temporal discretisation of the equation system is done by finite differences for the differentiation with respect to time with time step $\Delta t^j = t^{j+1} - t^j$ between time t^j and t^{j+1}:

$$\left(\omega \mathbf{A}^{j+1} + \frac{1}{\Delta t^j}\mathbf{B}^{j+1}\right)\ \widetilde{\mathbf{c}}^{j+1} = \left((1-\omega)\mathbf{A}^j + \frac{1}{\Delta t^j}\mathbf{B}^j\right)\ \widetilde{\mathbf{c}}^j\ +\ \mathbf{f}^j \tag{491}$$

This results in different discretisations depending on the choice of the parameter ω, e.g. we have for $\omega = 0$ the explicit method, for $\omega = \frac{1}{2}$ the Crank-Nicolson method and for $\omega = 1$ the fully implicit method.

To avoid numerical dispersion when applying the Crank-Nicolson mehod the dispersion coefficient is corrected using an approximation of third order for the time derivative (Huang et al., 1997):

$$D^- = D - \frac{q^2\,\Delta t}{6\,R\,\theta^2\varphi} \quad , \quad D^+ = D + \frac{q^2\,\Delta t}{6\,R\,\theta^2\,\varphi} \tag{492}$$

$$\text{with} \qquad \varphi = 1 + (n_f - 1)(1 - 1/R) \tag{493}$$

Thereby the correction at the new time level t^{j+1} is done by replacing D by D^- in the matrix $\omega\mathbf{A}^{j+1}$ and the correction at the old time level t^j by replacing D by D^+ in the matrix $(1-\omega)\mathbf{A}^j$ of equation (491).

Furthermore, to avoid numerical oscillations both in case of the Crank-Nicolson and also in case of the fully implicit method an 'upwinding' of the convection term is performed (Huang et al., 1997). This is achieved by evaluation of the terms A^q_{ij} in equation (491) where instead of the basis functions $\phi_i\ ,\ 1 \le i \le n$ the asymmetric functions

$$w_i = \begin{cases} \phi_i + 3\,\gamma^w_{i-1}\,\phi_{i-1}\,\phi_i & \text{on} \quad \Omega_{i-1} = [x_{i-1}, x_i] \\ \phi_i - 3\,\gamma^w_i\,\phi_i\,\phi_{i+1} & \text{on} \quad \Omega_i = [x_i, x_{i+1}] \end{cases} \tag{494}$$

for $1 < i \le n+1$ are used, where w_1 is defined only on Ω_1 and w_{n+1} only on Ω_n.

The weighting factor γ^w_i is determined by the Peclet number $Pe_i = q_i\ \Delta z/(\theta_i D_i)$ at each knot i:

$$\gamma^w_i = \coth\left(\frac{Pe_i}{2}\right) - \frac{2}{Pe_i} \quad . \tag{495}$$

If now the spatial step size Δz is chosen in such a way, that $Pe_i \le 2$ for all $1 \le i \le n$, then numerical oscillations are avoided.

Hence we get as expression for the term A^q_{ij}:

$$\begin{aligned} A^q_{ij} &= \sum_e \int_{\Omega_e} -q_w\,w_j \frac{dw_i}{dz}\,dz = \sum_{e=i}^{i+1} \int_{\Omega_e} \sum_{k=e-1}^{e} -q_k\,w_k\,w_j \frac{dw_i}{dz}\,dz = \\ &= \begin{cases} -(2q_{i-1} + q_i)/6 - \gamma^w_{i-1}/2\ \ q_{i-1} & \text{for } i-1=j \\ (q_{i+1} - q_{i-1})/6 + (\gamma^w_{i-1} + \gamma^w_i)/2\ \ q_i & \text{for } i=j \\ (q_i + 2q_{i+1})/6 - \gamma^w_i/2\ \ q_{i+1} & \text{for } i+1=j \\ \qquad 0 & \text{for } |i-k|>1 \end{cases} \end{aligned} \tag{496}$$

The consideration of these corrections leads to a tridiagonal system of equations, which is linear in case of a linear Freundlich isotherm, but otherwise represents a non-linear equation system. In the linear case the equation system is directly solved applying a LU-decomposition. In the non-linear case, the solution is obtained by a Picard fix-point iteration and a LU-decomposition in each iteration step.

The corresponding equation system is finally given by the following equation in matrix notation, s. also section 1.4.4.6:

$$\mathbf{P}^{j+1,k}\,\tilde{\mathbf{c}}^{j+1,k} = \mathbf{g}^{j} \tag{497}$$

$$\begin{aligned} \text{mit}\quad \mathbf{P}^{j+1,k} &:= \omega\mathbf{A}^{j+1} + \frac{1}{\Delta t^j}\mathbf{B}^{j+1} \quad , && (498)\\ \text{und}\qquad \mathbf{g}^{j} &:= \left((1-\omega)\mathbf{A}^{j} + \frac{1}{\Delta t^j}\mathbf{B}^{j}\right)\,\tilde{\mathbf{c}}^{j} + \mathbf{f}^{j} \quad , && (499)\end{aligned}$$

where in the case $\omega = \frac{1}{2}$ with respect to the dispersion, the matrices $\mathbf{A} * +1$ or $\mathbf{A}^j$ are corrected by inserting D^- or D^+.

Explicitly we have for $1 < i < n+1$:

$$\begin{aligned} P^{j+1,k}_{i,i-1} &= \frac{\Delta z}{12\,\Delta t^j}\,(\theta_{i-1}R^k_{i-1} + \theta_i R^k_i) - \frac{\omega}{2\Delta z}(\theta_{i-1}D_{i-1} + \theta_i D_i)\\ &\quad -\frac{\omega}{6}[(2+3\gamma^w_{i-1})q_{i-1} - q_i] && (500)\end{aligned}$$

$$\begin{aligned} P^{j+1,k}_{i,i} &= \frac{\Delta z}{12\,\Delta t^j}\,(\theta_{i-1}R^k_{i-1} + 6\,\theta_i R^k_i + \theta_{i+1}R^k_{i+1})\\ &\quad +\frac{\omega}{2\,\Delta z}(\theta_{i-1}D_{i-1} + 2\,\theta_i D_i + \theta_{i+1}D_{i+1})\\ &\quad +\frac{\omega}{6}[q_{i+1} + 3(\gamma^w_{i-1} + \gamma^w_i)q_i - q_{i-1}] && (501)\end{aligned}$$

$$\begin{aligned} P^{j+1,k}_{i,i+1} &= \frac{\Delta z}{12\,\Delta t^j}\,(\theta_i R^k_i + \theta_{i+1}R^k_{i+1}) - \frac{\omega}{2\Delta z}(\theta_i D_i + \theta_{i+1}D_{i+1})\\ &\quad +\frac{\omega}{6}[(2-3\gamma^w_i)q_{i+1} + q_i] \quad , && (502)\end{aligned}$$

where $\theta_i,\ R^k_i,\ D_i,\ q_i$ and γ^w_i denote the values at time t^{j+1}, and in case of $\omega = \frac{1}{2}$ the parameter D_i is replaced by D^-_i.

Finally, for $i = 1$ resp. $i = n + 1$ we have to describe the flux boundary conditions:

$$\begin{aligned} P_{1,1}^{j+1,k} &= \frac{\Delta z}{12\,\Delta t^j}\,(3\,\theta_1 R_1^k + \theta_2 R_2^k) + \frac{\omega}{2\,\Delta z}(\theta_1 D_1^- + \theta_2 D_2^-) \\ &\quad + \frac{\omega}{6}[q_2 + (2 + 3\gamma_2^w)q_1] \end{aligned} \tag{503}$$

$$\begin{aligned} P_{n+1,n+1}^{j+1,k} &= \frac{\Delta z}{12\,\Delta t^j}\,(\theta_n R_n^k + 3\,\theta_{n+1} R_{n+1}^k) + \frac{\omega}{2\,\Delta z}(\theta_n D_n^- + \theta_{n+1} D_{n+1}^-) \\ &\quad - \frac{\omega}{6}[(2 - 3\gamma_{n+1}^w)q_{n+1} + q_n] \end{aligned} \tag{504}$$

In the same way the elements of the matrix $\left((1-\omega)\mathbf{A}^j + \frac{1}{\Delta t^j}\mathbf{B}^j\right)$ are calculated, to obtain the vector $\mathbf{g}^j$. But in this case, the matrix elements represent values at time t^j and therefore are not iterated, and in case $\omega = \frac{1}{2}$ the values D_i are replaced by D_i^+.

3.2.7 Dual-Porosity Solute Transport following MUNETOS / Expert-N

A dual-porosity solute transport model was developed and implemented to simulate solute transport in soils that have distinct regions of mobile and immobile water. Based on the numerical Euler-Lagrange method a numerical solution similar to the method used in the model MUNETOS (Zurmühl, 1994; Zurmühl and Durner, 1996; Zurmühl, 1998) is derived.

3.2.7.1 Transport equations To directly consider the solute exchange between the mobile and immobile pore water regions and to describe the sink terms that can dominate N transport, the following, in comparison to Zurmühl (1994) and Zurmühl and Durner (1996) modified transport equations are applied:

$$(\theta_m + f\rho_s K_d)\frac{\partial c_m}{\partial t} \;=\; \frac{\partial}{\partial z}[\theta_m D_{I,m}\frac{\partial c_m}{\partial z}] - q_w\frac{\partial c_m}{\partial z} + \beta\,(c_m - c_{im}) - S_{c_m} \tag{505}$$

$$[\theta_{im} + (1-f)\rho_s K_d]\,\frac{\partial c_{im}}{\partial t} = \alpha\,(c_m - c_{im}) - S_{c_{im}} \tag{506}$$

with abbreviation

$$\beta = \frac{\partial \theta_{im}}{\partial t} + S_{w,im} - \frac{\partial f}{\partial t}\rho_s K_d - \alpha \tag{507}$$

$\theta_m = \theta_m(t,z)$	mobile volumetric water content $[mm^3\ mm^{-3}]$
$\theta_{im} = \theta_{im}(t,z)$	immobile volumetric water content $[mm^3\ mm^{-3}]$
$f = f(t,z)$	fraction of sorption sites in the mobile region [1], e.g.: $f = \frac{\theta_m}{\theta}$
$\rho_s = \rho_s(z)$	soil bulk density $[kg\ dm^{-3}]$
$c_m = c_{I,m}(t,z)$	concentration of solute in the mobile water phase $[mg\ dm^{-3}]$
$c_{im} = c_{I,im}(t,z)$	concentration of solute in the mobile water phase $[mg\ dm^{-3}]$
$D_{I,m} = D_I(\theta_m, q_w)$	dispersion coefficient $[mm^2\ d^{-1}]$ of chemical I
$q_w = q_w(t,z)$	vol. water flux $[mm\ d^{-1}]$
$K_d = K_{d,I}(z)$	equilibrium adsorption constant $[dm^3\ kg^{-1}]$
$\alpha = \alpha(z)$	solute transfer coefficient $[d^{-1}]$ between mobile and immobile region
$S_{w,m},\ S_{w,im}$	sinks/sources of mobile/immobile water phase $[d^{-1}]$
$S_{c_m},\ S_{c_{im}}$	sinks/sources of mobile/immobile solute $[mg\ dm^{-3}\ d^{-1}]$

The transport equations of the two regions result from the continuity equation of the water phase (92) for $\theta = \theta_m + \theta_{im}$:

$$\frac{\partial \theta_m}{\partial t} = -\,\frac{\partial q_w}{\partial z} \;-\; \frac{\partial \theta_{im}}{\partial t} \;-\; S_{w,m} \;-\; S_{w,im} \tag{508}$$

and from the general solute transport equation of the total soil volume:

$$\frac{\partial}{\partial t}\{(\theta_m{+}f\rho_s K_d)c_m + [\theta_{im}{+}(1{-}f)\rho_s K_d]c_{im}\} = \frac{\partial}{\partial z}[\theta_m D_{I,m}\frac{\partial c_m}{\partial z}{-}q_w\,c_m] + \Phi_I \tag{509}$$

with sink/source term $\Phi_I = -S_{w,m}c_m - S_{w,im}c_{im} - S_{c_m} - S_{c_{im}}$

By differentiation and inserting (508) into (509) results the following equation

$$\begin{aligned}(\theta_m + f\rho_s K_d)\frac{\partial c_m}{\partial t} &= \frac{\partial}{\partial z}[\theta_m D_{I,m}\frac{\partial c_m}{\partial z}] - q_w\frac{\partial c_m}{\partial z}\\ &+ (S_{w,im} + \frac{\partial \theta_{im}}{\partial t} - \frac{\partial f}{\partial t}\rho_s K_d)(c_m - c_{im}) \qquad (510)\\ &- [\theta_{im} + (1-f)\rho_s K_d]\,\frac{\partial c_{im}}{\partial t} + (\Phi_I + S_{w,m}c_m + S_{w,im}c_{im})\ ,\end{aligned}$$

from which the transport equation (505) is obtained by inserting the transfer equation (506).

3.2.7.2 Numerical solution To numerically solve the transport equation (505) together with equation (506) an Euler-Lagrange method in combination with grid adaptation following Yeh (1990) is applied. In addition, to calculate the solute concentration in the Lagrange step the generalized operator splitting approach of Zurmühl (1994) for the instationary case is chosen.

a) Lagrange step: The idea behind the Euler-Lagrange method is to split the convective part of the transport equation from the dispersive part by a transformation of coordinates (Lagrange step) and then to numerically solve the transformed equation that includes only the dispersive part. The transformation is based on a change of the reference system that is chosen in a way that the observer is moved with the effective velocity v_e $[mm\ d^{-1}]$ of a solute volume element (Lagrange perspective). The corresponding co-ordinate in space is then given by $z' = z + v_e t$.

Stationary case: Under stationary flow conditions we obtain for the total derivation of the concentration with respect to time:

$$\frac{dc}{dt} = \frac{\partial c}{\partial t} + \frac{\partial c}{\partial z'}\frac{\partial z'}{\partial t} = \frac{\partial c}{\partial t} + v_e\frac{\partial c}{\partial z'} \qquad (511)$$

This can be exploited by using the stationary constant velocity $v_e = \dfrac{q_w}{\theta_m + f\rho_s K_d}$ to transform the transport equation (505) into:

$$(\theta_m + f\rho_s K_d)\frac{\partial c_m}{\partial t} = \frac{\partial}{\partial z}[\theta_m D_{I,m}\frac{\partial c_m}{\partial z}] + \beta\,(c_m - c_{im}) - S_{c_m} \qquad (512)$$

The transformed equation then contains no convective term anymore and is to be solved by the Euler step. Yet first the concentration c_m^* after the Lagrange step, i.e. after accounting for convection, has to be determined at each spatial node i. This is achieved in the case of stationary flow at constant flow velocity v_e in a comparatively simple way:

$$c_{m,i}^* = c_m(z_i, t^{j+1}) = c_m(z_i^*, t^j) \quad \text{using} \quad z_i^* = z_i - v_e\Delta t^j \qquad (513)$$

z_i^* position of a virtual mass particle at time t^j, that reaches node z_i at time t^{j+1}
$c_{m,i}^*$ concentration at node i at time t^{j+1} after accounting for convection

In fact, z_i^* often does not coincide with any of the nodes z_i, but nevertheless $c_{m,i}^*$ can be determined by linear interpolation:

$$c_{m,i}^* = c_{m,i-1}^j + (v_e \Delta t^j - \sum_{k=1}^{l} \Delta z_{i-k}) \frac{c_{i-l-1}^j - c_{i-l}^j}{\Delta z_{i-l-1}} \tag{514}$$

whereby l is the number of nodes that a virtual particle traverses during the time interval Δt^j before it reaches node i with the velocity v_e. The number l being thereto determined by the following condition (particle tracking):

$$v_e \Delta t^j - \sum_{k=1}^{l} \Delta z_{i-k} \geq 0 \quad \text{and} \quad v_e \Delta t^j - \sum_{k=1}^{l+1} \Delta z_{i-k} \leq 0 \tag{515}$$

Instationary case: The operator splitting technique and the related numerical procedure as derived for the stationary case can be transfered to the instationary case by calculating the concentration c_m^* after the convective step using mass flux considerations (Zurmühl, 1994). The equation to be solved during the Lagrange step is the mass balance equation for the convective mass flux q_s^c:

$$\frac{\partial}{\partial t}[(\theta_m + f \rho_s K_d)\, c_m] \;=\; -\frac{\partial q_s^c}{\partial z} \tag{516}$$

Using a finite difference discretisation of (516) at each vertical node i the concentration $c_{m,i}^*$ after convection can be calculated by

$$c_{m,i}^* = \frac{c_{m,i}^j \theta_{m,i}^j R_{m,i}^j \Delta z_i - (q_{s,i+1}^c - q_{s,i}^c) \Delta t^j}{\theta_{m,i+1}^{j+1} R_{m,i+1}^{j+1} \Delta z_i} \tag{517}$$

with $R_{m,i}^j = 1 + f_i^j \rho_s K_d / \theta_{m,i}^j$ and the convective mass fluxes $q_{s,i}^c$ and $q_{s,i+1}^c$.

Exploiting the fact, that the Richards equation can be solved almost without any mass balance error, we have, given the sink term $S_i^j = S_{w,m,i}^j + S_{w,im,i}^j + (\theta_{im,i+1}^j - \theta_{im,i}^j)/\Delta t^j$, for each time step j and at each vertical node i :

$$\theta_{m,i}^j \Delta z_i = \theta_{m,i}^{j+1} \Delta z_i - q_{w,i}^{j+1} \Delta t^j + q_{w,i+1}^{j+1} \Delta t^j + S_i^j \Delta z_i \Delta t^j \tag{518}$$

This allows to determine the convective mass flux in analogy to the stationary case by a particle tracking method as follows:

Convective mass flux $q_{s,i}^c$: In case of volumetric water flow $q_{w,i}^{j+1} > 0$: Mass particles are to be considered that contribute to the mass flux in node i. Thereto, in similarity to conditions

(516), a number l_i has to be found by which the nodes that were traversed during time step Δt^j can be identified.

For this purpose a discrete function J_i is defined by

$$J_i(l) = q_{w,i}^{j+1}\Delta t^j - \sum_{k=1}^{l} Q_{i-k}^j \Delta z_{i-k} \tag{519}$$

and $Q_i^j = \theta_{m,i}^{\,j} R_{m,i}^j - S_i^j \Delta t^j$

Then, by using condition $\quad J_i(l_i - 1) > 0 \;$ and $\; J_i(l_i) < 0 \quad$ (520)

a number l_i is determined, such that the function J_i changes its sign between $l_i - 1$ and l_i.

The general procedure is the following: First the volume of soil solution $q_{w,i}^{j+1}\Delta t^j$ that was transported during time step Δt^j by the water flux $q_{w,i}^{j+1}$ into node i is compared to the volume $(\theta_{m,i-1}^{\,j} + f_{i-1}^j \rho_s K_d - S_{i-1}^j \Delta t^j)\Delta z_{i-1} = Q_{i-1}^j \Delta z_{i-1}$ at time j at node $i-1$ which includes sorption sites and the sink or source of water. If $q_{w,i}^{j+1}\Delta t^j < Q_{i-1}^j \Delta z_{i-1}$ then a virtual particle that is located in node i at time t^j can only come from node $i-1$. If $q_{w,i}^{j+1}\Delta t^j \geq Q_{i-1}^j \Delta z_{i-1}$ the particle comes from a node smaller as $i-1$. In this case the volume $q_{w,i}^{j+1}\Delta t^j$ is further compared with $Q_{i-1}^j \Delta z_{i-1} + Q_{i-2}^j \Delta z_{i-2}$, etc. Therefore the value $i - l_i$ denotes the node where the concentration at time t^j still influences the concentration of node i at time t^{j+1} (Zurmühl, 1994).

In this way the convective mass flux $q_{s,i}^c$ during Δ^j can be calculated by the total mass which is transported to node i during Δ^j using

$$q_{s,i}^c \Delta t^j = \sum_{k=1}^{l_i - 1} c_{m,i-k}^j Q_{i-k}^j \Delta z_{i-k} + [Q_{i-l_i}^j \Delta z_{i-l_i} + J_i(l_i)] c_{m,i-l_i}^j \tag{521}$$

or using the by means of (518) transformed equation

$$\begin{aligned} q_{s,i}^c \Delta t^j \;&=\; \sum_{k=1}^{l_i} c_{m,i-k}^j \theta_{m,i-k}^{j+1} R_{m,i-k}^* \Delta z_{i-k} + \sum_{k=1}^{l_i} c_{m,i-k}^j (q_{w,i-k+1}^{j+1} - q_{w,i-k}^{j+1}) \Delta t^j \\ &\quad + J_i(l_i) c_{m,i-l_i}^j \end{aligned} \tag{522}$$

with notation $\; R_{m,i}^* = 1 + f_i^j \rho_s K_d / \theta_{m,i}^{j+1}$.

For a negative water flux $q_{w,i}^{j+1} < 0$, equation (519) is transformed in the following way:

$$J_i(l) = -q_{w,i}^{j+1}\Delta t^j - \sum_{k=0}^{l} Q_{i+k}^j \Delta z_{i+k} \tag{523}$$

and l_i is again determined by condition (520). Thus, the mass flux $q^c_{s,i}$ is obtained by

$$\begin{aligned} q^c_{s,i}\Delta t^j &= \sum_{k=0}^{l_i} c^j_{m,i+k}\theta^{j+1}_{m,i+k}R^*_{m,i+k}\Delta z_{i+k} - \sum_{k=0}^{l_i} c^j_{m,i+k}(q^{j+1}_{w,i+k+1} - q^{j+1}_{w,i+k})\Delta t^j \\ &\quad + J_i(l_i)c^j_{m,i+l_i} \end{aligned} \tag{524}$$

Convective mass flux $q^c_{s,i+1}$: If $q^{j+1}_{w,i+1} > 0$, then the discrete function $J_{i+1}(l)$ can be defined as follows by:

$$J_{i+1}(l) = q^{j+1}_{w,i+1}\Delta t^j - \sum_{k=1}^{l} Q^j_{i-k}\Delta z_{i-k} \tag{525}$$

Now by the condition $\qquad J_{i+1}(l_{i+1} - 1) < 0 \;$ and $\; J_{i+1}(l_{i+1}) > 0 \qquad$ (526)

the number l_{i+1} is determined, by which under consideration of (518) the mass flux $q^c_{s,i+1}$ out of node i can be calculated:

$$\begin{aligned} q^c_{s,i+1}\Delta t^j &= \sum_{k=0}^{l_{i+1}} c^j_{m,i-k}\theta^{j+1}_{m,i-k}R^*_{m,i-k}\Delta z_{i-k} + \sum_{k=0}^{l_{i+1}} c^j_{m,i-k}(q^{j+1}_{w,i-k+1} - q^{j+1}_{w,i-k})\Delta t^j \\ &\quad + J_{i+1}(l_{i+1})c^j_{m,i-l_{i+1}} \end{aligned} \tag{527}$$

In case $q^{j+1}_{w,i+1} < 0$ we get in almost the same manner from

$$J_{i+1}(l) = -q^{j+1}_{w,i+1}\Delta t^j - \sum_{k=1}^{l} Q^j_{i+k}\Delta z_{i+k} \tag{528}$$

and the condition (526) the mass flux $q^c_{s,i+1}$:

$$\begin{aligned} q^c_{s,i+1}\Delta t^j &= \sum_{k=1}^{l_{i+1}} c^j_{m,i+k}\theta^{j+1}_{m,i+k}R^*_{m,i+k}\Delta z_{i+k} + \sum_{k=1}^{l_{i+1}} c^j_{m,i+k}(q^{j+1}_{w,i+k+1} - q^{j+1}_{w,i+k})\Delta t^j \\ &\quad + J_{i+1}(l_{i+1})c^j_{m,i+l_{i+1}} \end{aligned} \tag{529}$$

Alltogether, by knowing the convective mass fluxes at nodes i, $i+1$ and by means of the mass balance (517) the concentration $c^*_{m,i}$ after the convective step can be determined.

b) Euler step: After consideration of the convective part, in the next step, the Euler step, the remaining dispersion equation is numerically solved. For this purpose the transport equation (505) without convective term is discretized following a fully implicit finite difference scheme. Then, according to the first order operator splitting technique, instead of the concentration of the preceding time step c^j_m the concentration obtained after the Lagrange step c^*_m is inserted:

$$\theta^{j+1}_{m,i}R^{j+1}_{m,i}\frac{c^{j+1}_{m,i} - c^*_{m,i}}{\Delta t^j} = \theta^{j+1}_{m,i+\frac{1}{2}}D^{j+1}_{m,i+\frac{1}{2}}\frac{c^{j+1}_{m,i+1} - c^{j+1}_{m,i}}{(\Delta z_i)^2} - \theta^{j+1}_{m,i-\frac{1}{2}}D^{j+1}_{m,i-\frac{1}{2}}\frac{c^{j+1}_{m,i} - c^{j+1}_{m,i-1}}{(\Delta z_i)^2}$$

$$+\Big[\frac{\theta_{im,i}^{j+1}-\theta_{im,i}^{j}}{\Delta t^j}+S_{w,m,i}^{j}-\frac{f_i^{j+1}-f_i^{j}}{\Delta t^j}\rho_s K_d-\alpha_i\Big](c_{m,i}^{j+1}-c_{im,i}^{j+1})\ -\ S_{c_m,i}^{j} \tag{530}$$

Herein $c_{im,i}^{j+1}$ can be expressed in dependence of $c_{m,i}^{j+1}$ by use of the discretized form of the solute transfer equation (506):

$$[\theta_{im,i}^{j+1}+(1-f_i^{j+1})\rho_s K_d]\,\frac{c_{im,i}^{j+1}-c_{im,i}^{j}}{\Delta t^j}=\alpha_i(c_{m,i}^{j+1}-c_{im,i}^{j+1})-S_{c_{im},i}^{j} \tag{531}$$

The discretisation (530) results in a linear tridiagonal equation system of $n-2$ equations in the n unknowns $c_{m,i}^{j+1}$ $(1\le i\le n)$, that can be directly solved by taking account of the boundary conditions and using the Gauss elimination procedure, i.e. by LU-decomposition (cf. section 1.4.4.5).

c) Initial and boundary conditions The input and output of the chemical occurs via the convective flux is calculated in the Lagrange step by consideration of the corresponding water fluxes by specification of a Dirichlet bundary condition at the upper $z=0$ and lower $z=\ell$ boundary:

$$c_m^*(t,z)=c_0(t)\quad\text{for } z=0\qquad\text{bzw.}\quad c_m^*(t,z)=c_\ell(t)\quad\text{for } z=\ell \tag{532}$$

In the Euler step, that deals with the dispersive part of the transport equation, both at the upper $z=0$ and at the lower end $z=\ell$ of the soil profile a von Neumann boundary condition is given:

$$-\theta\,D\,\frac{\partial c_m}{\partial z}\bigg|_{z=0}\ =\ -\theta\,D\,\frac{\partial c_m}{\partial z}\bigg|_{z=\ell}\ =\ 0 \tag{533}$$

The discretization of these boundary conditions completes the equation system, that is solved to provide the numerical solution of the nonequilibrium transport equations.

3.2.7.3 Grid adaptation To avoid numerical dispersion in combination with the Euler-Lagrange method often a grid refinement is applied, since in contrast to the pure Euler discretization a time step refinement is not necessary. Since a grid refinement of the total considered transport domain is connected with high computational costs and numerical dispersion mostly occurcs in regions of steep concentration gradients, the grid is only refined near the concentration front. This is achieved using the procedure of the model LEZOOM Yeh (1990), by which the grid refinement 'moves' with the concentration front (Zurmühl, 1994).

3.2.8 Transport of Dissolved Organic Nitrogen (DON)

3.2.8.1 Transport Equation To model the transport of dissolved organic nitrogen (DON) it is assumed that also the transport of this N-fraction can be described by a convection-dispersion equation. Since additionally the often observed DON transport along preferential flow paths will be considered, an equation following the non-equilibrium approach given by van Genuchten and Wierenga (1976) will be applied. In analogy to the solute transport model of the model WAVE (Vanclooster et al., 1994), see equations (439) and (440), a dual-porosity solute transport model is proposed:

$$\frac{\partial}{\partial t}\,[\,(\theta_m + f\rho_s K_d)\,c_m\,] \;=\; \frac{\partial}{\partial z}[\,\theta_m D_{DON}\,\frac{\partial c_m}{\partial z} \;-\; q_w\,c_m\,] \;-\alpha\,(c_m - c_{im}) \;+\; S_{c,DON,m} \tag{534}$$

$$\frac{\partial}{\partial t}\,[\,(\theta_{im} + (1-f)\rho_s K_d)\,c_{im}\,] \;=\alpha\,(c_m - c_{im}) \;+\; S_{c,DON,im} \tag{535}$$

$\theta_m = \theta_m(t,z)$	mobile volumetric water content $[mm^3\ mm^{-3}]$
$\theta_{im} = \theta_{im}(t,z)$	immobile volumetric water content $[mm^3\ mm^{-3}]$
$f = f(z)$	fraction of sorption sites in the mobile region [1]
$\rho_s = \rho_s(z)$	soil bulk density $[kg\ dm^{-3}]$
$c_m = c_m(t,z)$	DON solute concentration in the mobile soil water $[mg\ dm^{-3}]$
$c_{im} = c_{im}(t,z)$	DON solute concentration in the immobile soil water $[mg\ dm^{-3}]$
$D_{DON} = D_{DON}(\theta_m, q_w)$	dispersion coefficient $[mm^2\ d^{-1}]$ zum DON
$q_w = q_w(t,z)$	vol. water flux $[mm\ d^{-1}]$
$S_{c,DON,m}$	sink term $[mg\ dm^{-3}\ d^{-1}]$ of the mobile fraction
$S_{c,DON,im}$	sink term $[mg\ dm^{-3}\ d^{-1}]$ of the immobile fraction
$K_d = K_{d,DON}(z)$	equilibrium adsorption constant of DON $[dm^3\ kg^{-1}]$
$\alpha = \alpha(z)$	exchange coefficient $[d^{-1}]$ between mobile and immobile region

If only negligible amounts of immobile water exists and therefore the total water content θ can be assumed to be mobile, i.e. if $\theta_m = \theta$, then equation (534) reduces to the usual convection-dispersion equation (422) and equation (535) for the immobile soil solution is not needed.

If a constant C/N-ratio for the dissolved organic matter is assumed, the transport equations (534) and (535) represent also transport equations for dissolved organic carbon (DOC) except for possibly different sink terms. Under certain conditions on the sink terms, the calculated C/N-ratio of the dissolved organic matter stays constant such that from the simulated DON transport also the DOC transports results. If these conditions are not fulfilledand the C/N-ratio of dissolved organic matter is not constant, then similar equations as given by (534) and (535) are applied for the simulation of DOC transport.

3.2.8.2 Sink Terms The sink terms $S_{c,DON,i}$ for the mobile ($i = m$) and the immobile ($i = im$) pore-region, that describe the loss resp. the gain of DON during solute transport, are given by the following corresponding first order rates:

$$\begin{aligned} S_{c,DON,i} &= \theta_i/\theta \; (k_{hum,DON} N_{hum} + k_{lit,DON} N_{lit} + k_{man,DON} N_{man}) \; e_\theta \; e_T \\ &\quad - (k_{DON,hum} + k_{DON,lit} + k_{DON,min}) \; e_\theta \; e_T \; c_i, \quad i = m, im \end{aligned} \tag{536}$$

$S_{c,DON,i}$	sink term $[mg\ dm^{-3}\ d^{-1}]$ of the mobile ($i = m$) or immobile ($i = im$) region
θ_i	mobile ($i = m$) or immobile ($i = im$) vol. water content $[mm^3\ mm^{-3}]$
θ	total volumetric water content $[mm^3\ mm^{-3}]$
$k_{hum,DON}$	constant first order decomposion rate of humus-N to DON $[d^{-1}]$
N_{hum}	amount of soil humus-N $[kg\ ha^{-1}]$
$k_{lit,DON}$	constant first order decomposion rate of litter N to DON $[d^{-1}]$
N_{lit}	amount of N in the litter pool $[kg\ ha^{-1}]$
$k_{man,DON}$	constant first order decomposion rate of manure N to DON $[d^{-1}]$
N_{man}	amount of N in the manure pool $[kg\ ha^{-1}]$
e_θ	reduction function of water content [1]
e_T	reduction function of temperature [1]
$k_{DON,hum}$	constant first order immobilisation rate of DON to humus-N $[d^{-1}]$
$k_{DON,lit}$	constant first order immobilisation rate of DON to litter N $[d^{-1}]$
$k_{DON,min}$	constant first order mineralisation-immobilisation rate of DON $[d^{-1}]$
$c_i = c_i(t, z)$	DON concentration in the mobile ($i = m$) or immobile ($i = im$) soil solution $[mg\ dm^{-3}]$

The mineralisation-immobilisation rate $k_{DON,min}$ $[d^{-1}]$ is defined similar to the approach of modelling mineralisation in the model SOILN, s. equation (591):

$$k_{DON,min} = (f_{C/N,DON}^{-1} - \frac{f_{e,DON}}{r_{0,DON}}) \; k_{DOC,min} \; f_{C/N,DON} \tag{537}$$

$k_{DON,min}$	constant first order mineralisation-immobilisation rate of DON $[d^{-1}]$
$k_{DOC,min}$	constant first order mineralisation rate of DOC $[d^{-1}]$
$f_{C/N,DON}$	C/N-ratio of dissolved organic matter [1]
$f_{e,DON}$	effectivity constant of DON-mineralising soil micro-organisms [1]
$r_{0,DON}$	C/N-ratio of DON-mineralising soil micro-organisms [1]

3.3 Urea-Hydrolysis, Nitrification and Volatilisation

Nitrification refers to the process of oxidation of ammonium into nitrate. It is a transformation process carried out by soil micro- organisms under aerobic conditions. The main factors affecting the nitrification are the ammonium pool N_{NH} $[kg\ ha^{-1}]$ within the soil, the available oxygen in soil air and soil solution, the pH value of the soil and the soil temperature.

3.3.1 Approaches of the model LEACHN

3.3.1.1 Urea-Hydrolysis To describe urea hydrolysis a sink term Φ_{HS} is defined for every numerical soil layer to represent the urea-N transformation to ammonium-N by soil microorganisms:

$$\Phi_{HS} = k_{HS}\ (\theta + \rho_s K_{d,HS})\ c_{HS}\ e_\theta\ e_T \tag{538}$$

Φ_{HS}	sink term of urea-hydrolysis $[mg\ dm^{-3}\ d^{-1}]$
k_{HS}	decomposition rate of urea $[d^{-1}]$
c_{HS}	urea-N concentration in the soil solution $[mg\ dm^{-3}]$
$K_{d,HS}$	adsorption coefficient of urea $[dm^3 kg^{-1}]$
θ	volumetric water content $[mm^3\ mm^{-3}]$
ρ_s	soil bulk density $[kg\ dm^{-3}]$
e_θ	reduction function of water content [1]
e_T	reduction function of soil temperature [1]

The reduction functions e_θ and e_T describe for every numerical soil layer the effects of the abiotic factors vol. water content and soil temperature on the nitrogen transformation processes, which are mainly driven by microbial activity (Johnsson et al. 1987). The reduction function e_θ of water content decreases at dry or very wet soil at both sides of a range of vol. soil water contents, which are optimal for the considered transformation rate:

$$e_\theta = \begin{cases} e_{sat} + (1 - e_{sat})\ (\theta_{sat} - \theta)/(\theta_{sat} - \theta_h) & \text{for } \theta_h < \theta \le \theta_{sat} \\ 1 & \text{for } \theta_l \le \theta \le \theta_h \\ [\max(\theta; \theta_w) - \theta_w]/(\theta_l - \theta_w) & \text{for } \theta < \theta_l \end{cases} \tag{539}$$

e_{sat}	reduction factor at water saturation [1]
θ_{sat}	saturated vol. water content $[mm^3\ mm^{-3}]$ set equal to the soil porosity
θ_w	minimal water content $[mm^3\ mm^{-3}]$ at which no N-transformation occurs anymore
θ_l	lower value of the optimal water content range $[mm^3\ mm^{-3}]$
θ_h	upper value of the optimal water content range $[mm^3\ mm^{-3}]$

The reduction function e_T of the temperature impact on the N-transformations is given by a Q_{10}-temperature function. The Q_{10}-value indicates the factor by which the N-Transformation rate changes at an increase or decrease in soil temperature of $10°C$:

$$e_T = Q_{10}^{0,1(T-T_B)} \tag{540}$$

e_T	reduction function of temperature $[1]$
T	soil temperature $[°C]$
T_B	base temperature $[°C]$ at which the rate of the N-transformation is determined
Q_{10}	Q10-factor $[1]$

3.3.1.2 Nitrification For ammonium-N the source or sink term Φ_{NH} per soil layer is composed from the source terms by urea-N Hydrolysis Φ_{HS} and N-mineralisation Φ_{MinNH} from fresh organic matter, humus, and organic fertilizers, as well as from sinks by N-immobilisation Φ_{ImmNH} due to fresh organic matter input, by nitrification Φ_{Nit}, by ammonium-N uptake of plant roots Φ_{WNH}, and in case of the upper soil layer by gaseous losses due to ammonia volatilisation Φ_{Vol}:

$$\Phi_{NH} = \Phi_{HS} + \Phi_{MinNH} - \Phi_{ImmNH} - \Phi_{Nit} - \Phi_{WNH} - \Phi_{Vol} \tag{541}$$

Here the sink of nitrification Φ_{Nit} per soil layer is identical to the nitrification rate k_{Nit} of the soil layer given by:

$$\Phi_{Nit} = k_{Nit} = k_{Nit,max}\ \max\{0,0; [c_{NH}\ (\theta + \rho_s K_{d,NH}) - c_{NO}\ \theta / r_{max}]\}\ e_\theta\ e_T \tag{542}$$

as described by Johnsson et al. (1987), where

Φ_{Nit}	sink term of nitrification $[mg\ dm^{-3}\ d^{-1}]$
k_{Nit}	nitrification rate $[mg\ dm^{-3}\ d^{-1}]$
$k_{Nit,max}$	maximal nitrification rate constant $[d^{-1}]$
c_{NH}	concentration of ammonium-N in the soil solution $[mg\ dm^{-3}]$
θ	volumetric water content $[mm^3\ mm^{-3}]$
ρ_s	soil bulk density $[kg\ dm^{-3}]$
$K_{d,NH}$	adsorption coefficient of ammonium $[dm^3\ kg^{-1}]$
c_{NO}	concentration of nitrate-N in the soil solution $[mg\ dm^{-3}]$
r_{max}	maximal ratio of Nitrat-N to ammonium-N $[1]$ at which no nitrification occurs anymore
e_θ	reduction function of water content $[1]$ according to equation (539)
e_T	reduktion function of temperature $[1]$ according to equation (540)

3.3.1.3 Volatilisation For the upper most 10 cm thick soil layer the ammonia-N volatilisation is calculated by:

$$\Phi_{Vol} = k_{Vol}\, c_{NH,1}\, \theta_1 \tag{543}$$

Φ_{Vol}	sink by ammonia-N volatilisation $[mg\ dm^{-3}\ d^{-1}]$
k_{Vol}	ammonia-N volatilisation rate $[d^{-1}]$
$c_{NH,1}$	ammonium-N concentration in the soil solution of the upper most soil layer $[mg\ dm^{-3}]$
θ_1	volumetric water content of the upper most soil layer $[mm^3\ mm^{-3}]$

where it is assumed, that within one day not more than half of the dissolved ammonium can escape from the soil.

The sink or source terms Φ_{MinNH}, Φ_{ImmNH}, and Φ_{WNH} are explained in more detail within the sections on mineralisation, immobilisation and on nitrogen uptake by plant roots.

3.3.2 Approaches of the model CERES-N

3.3.2.1 Urea-Hydrolysis To simulate urea hydrolysis, a maximum first order hydrolysis rate is estimated for each soil layer from the organic carbon content C_{org} $[kg\ ha^{-1}]$ and the pH-value of the layer:

$$k_{HS} = \min(0,25; -1,12\ +\ 1,13\, C_{org}\ +\ 0,203\, v_{pH} - 0,155\, C_{org}\, v_{pH}) \tag{544}$$

k_{HS}	hydrolysis rate $[d^{-1}]$ of the soil layer
C_{org}	organic carbon content $[kg\ ha^{-1}]$ of the soil layer
v_{pH}	pH value $[1]$ of the soil layer

For each soil layer then results the actual hydrolysis rate per day and hence the sink due to urea-N decomposition in the soil layer Φ_{HS} $[kg\ ha^{-1}d^{-1}]$ by multiplying with the minimum of the reduction functions of temperature f_T $[1]$ and moisture f_θ $[1]$ and considering the amount of urea-N N_{HS} $[kg\ ha^{-1}]$ present in the soil layer:

$$\Phi_{HS} = k_{HS}\ \min(f_T; f_\theta)\ N_{HS} \tag{545}$$

where the reduction function f_T $[1]$ of soil temperature T $[^\circ C]$ is given by

$$f_T = \max(T/40, 0^\circ\mathrm{C} + 0,2;\ 0,0) \tag{546}$$

and the reduction function of soil moisture f_θ [1] results from

$$f_\theta = \min[\max(\alpha; 0,0) + 0,2;\ 1,0] \tag{547}$$

and

$$\alpha = \begin{cases} (\theta - 0,5\,\theta_{pwp})/(\theta_{fc} - 0,5\,\theta_{pwp}) & \text{for } \theta \le \theta_{fc} \\ 1,0 - 0,5\,(\theta - \theta_{fc})/(\theta_{max} - \theta_{fc}) & \text{for } \theta > \theta_{fc} \end{cases} \tag{548}$$

θ	actual vol. water content $[mm^3\ mm^{-3}]$
θ_{fc}	vol. water content at field capacity $[mm^3\ mm^{-3}]$
θ_{pwp}	vol. water content at permanent wilting point $[mm^3\ mm^{-3}]$
θ_{max}	maximal vol. water content $[mm^3\ mm^{-3}]$, see eq. (486).

The amount of nitrogen released by urea hydrolysis is added to the ammonium-nitrogen pool of the respective soil layer. After 21 days, the remaining urea-N stock is considered to be completely hydrolysed and is also added to ammonium-N.

3.3.2.2 Nitrification The Ammonium-sink Φ_{Nit} $[kg\ ha^{-1}\ d^{-1}]$ due to nitrification is modelled per soil layer by a nitrification rate k_{Nit} $[kg\ ha^{-1}\ d^{-1}]$, which is controlled by Michaelis-Menten kinetics dependent on the ammonium-N mass fraction in the soil layer c_{NH} [mg N/kg soil]:

$$\Phi_{Nit} = k_{Nit} = k_{Nit,max}\ f_{Nit}\ c_{NH}/(c_{NH} + K_{Nit})\ N_{NH} \tag{549}$$

Φ_{Nit}	ammonium-N sink by nitrification $[kg\ ha^{-1}\ d^{-1}]$
k_{Nit}	nitrification rate $[d^{-1}]$
N_{NH}	ammonium-N amount in the soil layer $[kg\ ha^{-1}]$
c_{NH}	ammonium-N fraction in the soil layer $[mg\ kg^{-1}]$
K_{Nit}	Michaelis-Menten or half-saturation constant (=90,0) $[mg\ kg^{-1}]$
$k_{Nit,max}$	relativ maximal nitrification rate (=40,0) $[d^{-1}]$
f_{Nit}	reduction function of nitrification [1]

The reduction function of nitrification f_{Nit} [1] is here the minimal value of the moisture reduction factor f_θ [1], the temperature reduction factor f_T [1], the pH value f_{pH} and the relative nitrification potential $NitP$ [1]:

$$f_{Nit} = \min(f_\theta; f_T; f_{pH}; NitP) \tag{550}$$

The moisture reduction factor of nitrification results from:

$$f_\theta = \begin{cases} (\theta - \theta_{pwp})/(\theta_{fc} - \theta_{pwp}) & \text{for } \theta \leq \theta_{fc} \\ 1,0 \; - \; (\theta - \theta_{fc})/(\theta_{max} - \theta_{fc}) & \text{for } \theta > \theta_{fc} \end{cases} \tag{551}$$

θ	actual vol. water content $[mm^3 \; mm^{-3}]$
θ_{fc}	vol. water content at field capacity $[mm^3 \; mm^{-3}]$
θ_{pwp}	vol. water content at permanent wilting point $[mm^3 \; mm^{-3}]$
θ_{max}	maximal vol. water content $[mm^3 \; mm^{-3}]$, see eq. (486).

The temperature reduction factor f_T [1] is calculated from the soil temperature T $[^\circ C]$ by:

$$f_T = \max(T/30^\circ\mathrm{C}; \; 0,0) \tag{552}$$

The pH factor is determined by

$$f_{pH} = \begin{cases} (pH \; - \; 4,5)/1,5 & \text{for } pH \; < \; 6,0 \\ 1,0 & \text{for } 6,0 \leq pH \leq 8,0 \\ 9,0 \; - \; pH & \text{for } pH \; > \; 8,0 \end{cases} \tag{553}$$

and the relative nitrification potential $NitP$ [1] is estimated from the nitrification potential of the day before $NitP_{alt}$ [1] by

$$NitP = NitP_{alt} \; \exp[2,302 \; \min(f_c; f_T; f_\theta)] \tag{554}$$

where the concentration factor f_c [1], which describes a nitrification inhibition due to low ammonium concentration c_{NH} [mg N/kg Boden] is defined by

$$f_c = 1,0 \; - \; \exp(-0,01363 \; c_{NH}) \tag{555}$$

The nitrified ammonium-N is added to the nitrate-N pool of the soil, the intermediate step of nitrite production is not modeled.

3.3.3 N_2O-production during nitrification according to EXPERT-N

To quantify the production of N_2O during nitrification, it is assumed that the N_2O-production rate is directly proportional to the nitrification rate, where the nitrification in EXPERT-N is modeled as in the LEACHN model by first order kinetics.
Therefore, the N_2O-production rate during nitrification k_{Nit,N_2O} $[mg \; dm^{-3} \; d^{-1}]$ is given by

$$k_{Nit,N_2O} \; = \; \beta \, k_{Nit} \quad , \tag{556}$$

where $\beta = 0,01$ [1] represents the constant proportionality factor and k_{Nit} $[mg \; dm^{-3} \; d^{-1}]$ denotes the nitrification rate, see also equation (542).

3.4 Denitrification

Denitrification is the dissimilatory reduction of nitrate via nitrite to the gaseous compounds $NO,\ N_2O$ and N_2. It is a microbial process which takes place under anaerobic conditions, when microbes utilize oxidized nitrogen compounds as a terminal electron acceptor. The process is influenced by the organic carbon content, the oxygen supply, the temperature and the pH value of the soil.

3.4.1 Approaches of the models SOILN and LEACHN

The source- and sink-term of nitrate Φ_{NO} is obtained from the source by nitrification Φ_{Nit} and the sinks by immobilisation Φ_{ImmNO} , by nitrate uptake by plant roots Φ_{WNO} (root-nitrate uptake) and by denitrification Φ_{Den} :

$$\Phi_{NO} = \Phi_{Nit} - \Phi_{ImmNO} - \Phi_{WNO} - \Phi_{Den} \tag{557}$$

The process of denitrification is calculated per soil layer by the model SOILN according to

$$\Phi_{Den} = k_{Den}\ c_{NO}/[c_{NO} + K_{NO}]\ e_{\theta,Den}\ e_T \tag{558}$$

resp. by the model LEACHN from

$$\Phi_{Den} = k_{Den}\ c_{NO}^2/[c_{NO} + K_{NO}]\ e_{\theta,Den}\ e_T \tag{559}$$

Φ_{Den}	nitrat-N sink by denitrification $[mg\ dm^{-3}\ d^{-1}]$
k_{Den}	denitrification rate $[d^{-1}]$
c_{NO}	nitrate concentration in soil solution $[mg\ dm^{-3}]$
K_{NO}	half saturation constant or Michaelis-Menten constant $mg\ dm^{-3}]$
$e_{\theta,Den}$	reduction function of water content $[1]$ for the denitrification rate
e_T	reduction function of soil temperature $[1]$ for the denitrification rat according to eq. (541),

where the reduction function of water content $e_{\theta,Den}$ is defined by:

$$e_{\theta,Den} = \max\{0,0;\ [(\theta - 0,6\ \theta_{sat})/(\theta_{sat} - 0,6\ \theta_{sat})]\}^2, \tag{560}$$

and θ_{sat} denotes the saturated volumetric water content $[mm^3\ mm^{-3}]$ here assumed to be identical to the porosity of the soil layer. By the model LEACHN the denitrification rate, as defined for the model SOILN (Johnsson et al., 1987), is conceived as a rate constant of first order kinetics to describe denitrification. It is therefore additionally multiplied by the nitrate concentration.

Furthermore, it is assumed that denitrification per day can consume only a maximum of 10% of the carbon available from fresh organic matter, humus and organic fertilizer. The remaining sinks Φ_{ImmNO} and Φ_{WNO} are explained in the sections on mineralisation and immobilisation, as well as on nitrogen uptake by plants.

3.4.2 Approaches of the model CERES-N

By the models CERES-N (Godwin and Jones 1991) and N-SIM (Engel 1991) denitrification is only calculated, if the actual soil water content exceeds the water content at field capacity, if the soil temperature is higher than $1,0°\mathrm{C}$ and the nitrate amount within the soil layer is above 1,0 mg/kg soil. The nitrate-N sink by denitrification Φ_{Den} $[kg\ ha^{-1}\ d^{-1}]$ per soil layer results from the denitrification rate k_{Den} $[d^{-1}]$, a first order rate, and the nitrate-N content N_{NO} $[kg\ ha^{-1}]$ of the soil layer. The denitrification rate k_{Den} $[d^{-1}]$ itself is composed by the reduction functions of soil temperature f_T $[1]$ and of water content $f_\theta[1]$ and by the content of dissolved organic carbon C_{DOC} $[mg\ kg^{-1}]$ as well as by the optimal rate $k_{Den,max}$ $(= 6,0\ 10^{-5} mg^{-1}\ kg\ d^{-1})$:

$$\Phi_{Den} = k_{Den}\ N_{NO} = 6,0\ 10^{-5}\ f_T\ f_\theta\ C_{DOC}\ N_{NO} \tag{561}$$

For this formula the reduction functions are calculated in case of soil temperature T $[°C]$ by

$$f_T = 0,1\ \exp(0,046\ T) \tag{562}$$

and in case of volumetric soil water content θ $[mm^3\ mm^{-3}]$ by

$$f_\theta = 1,0\ -\ (\theta_{max} - \theta)/(\theta_{max} - \theta_{fc}) \tag{563}$$

f_θ	reduction factor fo water content for denitrification $[1]$
θ_{max}	maximal vol. water content of the soil layer $[mm^3\ mm^{-3}]$
θ	actual vol. water content of the soil layer $[mm^3\ mm^{-3}]$
θ_{fc}	vol. water content at field capacity $[mm^3\ mm^{-3}]$ of the soil layer

and further the dissolved organic carbon content C_{DOC} $[mg\ kg^{-1}]$ is estimated by

$$C_{DOC} = 24,5\ +\ 0,31\ (0,58\ C_{HUM}\ +\ 0,4\ C_{KH})/(\rho_s\ \Delta z) \tag{564}$$

C_{DOC}	dissolved organic carbon content of the soil layer $[mg\ kg^{-1}]$
C_{HUM}	carbon content of the stable organic matter pool (humus pool) $[kg\ ha^{-1}]$ of the soil layer
C_{KH}	carbo-hydrates of the pool of fresh organic matter (FOM) $[kg\ ha^{-1}]$ of the soil layer
ρ_s	soil bulk density of the soil layer $[kg\ dm^{-3}]$
Δz	thickness of the soil layer $[mm]$

3.4.3 Approaches of the model EXPERT-N

Instead of describing the denitrification as a single process, it can also be simulated in two steps as a reduction from nitrate to N_2O and as a subsequent reduction from N_2O to N_2. This is the concept followed by the model EXPERT-N. Also in this case, the nitrate reduction to the intermediate product nitrite and the NO formation occurring during this process are not directly taken into account here either, only the N_2O-production is explicitly described as a sub-process of denitrification.

3.4.3.1 N_2O Production The N_2O production rate k_{den,N_2O} $[mg\ dm^{-3}\ d^{-1}]$ during denitrification in the respective soil layer is estimated by the following equation:

$$k_{den,N_2O} = k_{den,N_2O,max}\ e_{\theta,d}\ e_{NO_3}\ e_T \tag{565}$$

k_{den,N_2O}	N_2O production rate during denitrification $[mg\ cm^{-3}\ d^{-1}]$		
$k_{den,N_2O,max}$	maximal N_2O production rate during denitrification $[mg\ cm^{-3}\ d^{-1}]$		
$e_{\theta,d}$	red.-fct. of water content [1]	e_{NO_3}	red.-fct. of nitrate content [1]
e_T	red.-fct. of soil temperature [1]		

The reduction function $e_{\theta,d}$ $[1]$ of volumetric water content θ here represents the availability of soil oxygen (O_2) (Johnsson et al., 1987), see also equation (560): At good aeration of the soil, the O_2 diffusion from the atmosphere into the soil air is not impeded. If, however, the air-carrying pores of the soil are increasingly filled with water, O_2 must diffuse through water films. This slows down the O_2 transport into the soil considerably, since the O_2 diffusion coefficient in water compared to that in air is much lower, approximately by the factor 10^{-5}. Therefore, at high water contents above a certain threshold value θ_d, low O_2 concentrations occur in the soil, in particular if the O_2 consumption due to the respiration of soil microorganisms and plants is higher than the then lower O_2 replenishment.

This fact is described by the function $e_{\theta,d}$. Below θ_d it is zero, i.e. the soil is well supplied with O_2 and there is no denitrification. Above the limit, the O_2-concentration is lower, denitrification may occur and with increasing water content, N_2O production may increase:

$$e_{\theta,d} = \left[\max\left(\frac{(\theta - \theta_d)}{(\theta_{sat} - \theta_d)}, 0\right)\right]^2 \tag{566}$$

$e_{\theta,d}$	reduction function of water content [1]		
θ_d	vol. water content-limit value of denitrification $[mm^3\ mm^{-3}]$		
θ_{sat}	saturated vol. water content $[mm^3\ mm^{-3}]$	θ	vol. water content $[mm^3\ mm^{-3}]$.

The possible limitation of the N_2O-production by low availability of soil nitrate-N is represented by the following reduction function of nitrate e_{NO_3}. It is given by an half-saturation constant K_{NO_3} $[mg\ dm^{-3}]$ of the nitrate-N concentration in soil solution:

$$e_{NO_3} = \frac{\theta\ c_{NO_3}}{\theta\ c_{NO_3} + K_{NO_3}} \tag{567}$$

e_{NO_3}	red.-fct. of nitrate-N content [1]	θ	vol. water content $[mm^3\ mm^{-3}]$
c_{NO_3}	nitrate-N concentration $[mg\ dm^{-3}]$ in soil solution		
K_{NO_3}	half saturation constant of of nitrat-N for N_2O-production $[mg\ dm^{-3}]$.		

Finally the impact of soil temperature T [°C] on the N_2O-production rate is modelled using the function e_T [1], which is defined by the following equation

$$e_T = Q_{10}^{(T-T_B)/10} \tag{568}$$

for a given Q_{10}-value [1] and a given base temperature T_B [°C].

3.4.3.2 N_2O-Reduction to N_2 The further reduction of N_2O to N_2 is described depending on the chosen N_2O-transport model. For the simpler model it is assumed, that the N_2O amount of the net N_2O production within the total soil profile is emitted immediately to the atmosphere. In this case the reduction rate k_{red,N_2} of N_2O to N_2 $[mg\ dm^{-3}\ d^{-1}]$ is defined assuming a direct proportionality to the net N_2O-production rate k_{den,N_2O} $[mg\ dm^{-3}\ d^{-1}]$ by a proportionality factor γ [1] (**constant N_2 to N_2O ratio**):

$$k_{red,N_2} = \gamma\ k_{den,N_2O} \tag{569}$$

The net-N_2O-emission rate Φ_{em,N_2O} $[mg\ m^{-2}]$ from the soil profile of depth ℓ $[mm]$ results then from:

$$\Phi_{em,N_2O} = \int_{z=\ell}^{z=0} k_{den,N_2O}\ (1-\gamma)\ dz\ \ . \tag{570}$$

If the more complex N_2O-transport model is chosen, which is based on a convection-dispersion equation, the reduction of N_2O to N_2 can be described by a first order reaction. The resulting N_2 to N_2O ratio then in general is not any more constant (**variable N_2 to N_2O ratio**). The reduction rate k_{red,N_2} of N_2O to N_2 $[mg\ dm^{-3}\ d^{-1}]$ is then defined as follows:

$$k_{red,N_2} = k_{red,N_2,max}\ e_{\theta,d}\ e_T\ e_I\ \theta\ K_H\ c_{N_2O} \tag{571}$$

$k_{red,N_2,max}$	maximal reduction rate of N_2O to N_2 $[mg\ dm^{-3}\ d^{-1}]$		
c_{N_2O}	N_2O-N concentration $[mg\ dm^{-3}]$ in soil air		
K_H	Henry constant of N_2O which represents the N_2O distribution coefficient between the gaseous and the liquid phase of N_2O in the soil [1]		
$e_{\theta,d}$	red.-fct. of water content [1]	e_{NO_3}	red.-fct. of nitrate content [1]
e_T	red.-fct. of soil temperature [1]	θ	vol. water content $[mm^3\ mm^{-3}]$

Here, the functions $e_{\theta,d}$ and e_T are the same as for the N_2O-production rate. Whereas the function e_I [1], which represents the effect of inhibition on the reduction of N_2O to N_2 at very high nitrate solute concentrations, is described by the following approach:

$$e_I = \frac{I_{NO_3}^3}{(\theta\ c_{NO_3})^3 + I_{NO_3}^3} \tag{572}$$

c_{NO_3} nitrate-N concentration in soil solution $[mg\ dm^{-3}]\theta$ vol. water content $[mm^3\ mm^{-3}]$
I_{NO_3} inhibition constant for N_2O-production $[mg\ dm^{-3}]$ of nitrate-N .

3.4.3.3 Frost-Thaw Effect In winter, under the influence of intense frost-thaw cycles, strongly increased N_2O releases may occur (Flessa et al., 1995; Kaiser and Heinemeyer, 1996; Mosier et al., 1996). The causes for the N_2O emissions from frost and thaw events are not yet fully clarified. On the one hand N_2O, which is formed in deeper soil and possibly accumulates under an ice layer may be set free during a thawing phase (Goodroad and Keeney, 1984; Burton and Beauchamps, 1994), on the other hand, death of microbial biomass and the destruction of soil aggregates may lead to increased release of easily available carbon and nitrogen compounds and hence to increased microbial activity (Christensen and Tiedje, 1990; Christensen and Christensen, 1991). In the model EXPERT-N it is assumed that the increased winter emissions are mainly caused by an increased N_2O production rate during denitrification, as the thawing phases most often lead to high water contents in the topsoil. Since the pursued model approach however is very simple, in the end it will not be distinguished between the release of newly formed or the release of possibly enclosed accumulated N_2O amounts. The increased N_2O release will be modeled by an increase in the N_2O production rate by use of an amplification function of thawing e_{thw} [1] in analogy to reduction functions. For this, it is assumed that e_{thw} is directly proportional to the change rate of the ice content θ_{ice} [1] in the soil, which is negative during thawing, when the ice content decreases:

$$e_{thw} = C_{thw}\ \max\Big(- \frac{\partial \theta_{ice}}{\partial t}, 0\Big) \tag{573}$$

C_{thw} amplification factor of the amplification function [1]

Thus we finally get the extended model for the N_2O-production rate during denitrification:

$$k_{den,N_2O} = k_{den,N_2O,max}\ e_{\theta,d}\ e_{NO_3}\ e_T\ (1 + e_{thw}) \tag{574}$$

k_{den,N_2O}	N_2O-production rate during denitrification $[mg\ cm^{-3}\ d^{-1}]$		
$k_{den,N_2O,max}$	maximal N_2O-production rate during denitrification $[mg\ cm^{-3}\ d^{-1}]$		
$e_{\theta,d}$	red.-fct. of water content [1]	e_{NO_3}	red.-fct. of nitrate content [1]
e_T	red.-fct. of soil temperature [1]	e_{thw}	amplification fct. of thawing [1]

3.4.3.4 Rewetting Effect To be able to describe the observed increase of N_2O emissions, as it occurs if the soil is rewetted after a longer time period without noteworthy rainfall events (Mosier and Hutchinson, 1981; Cates and Keeney, 1987; Hansen et al., 1993; de Klein and van Logtestijn, 1994; Flessa et al., 1995), the N_2O production model was further extended. It is assumed that the rewetting effect is triggered during more heavy rains of more than 10 mm water column per m^2 and that the effectiveness of a rewetting event on the N_2O production and denitrification depends on the last rewetting cycle that occurred. This dependency is represented by a measure F [mm] that indicates the drying of the soil by the cumulative potential evapotranspiration ET [mm] minus the cumulative Rainfall N [mm] since the last rewetting:

$$F(t_j) = \int_{t_{j-1}}^{t_j} ET(t) - N(t)\, dt \tag{575}$$

where t_j [d] denotes the actual time and t_{j-1} [d] the time of the last rewetting event. The maximal effectiveness factor of rewetting $f_{rew,max}$ [1] at time t_j is then given by:

$$f_{rew,max}(t_j) = min(\frac{F(t_j)}{F_{rew,max}}, 1) \tag{576}$$

where $F_{rew,max} = 20$ [mm] denotes the cumulative potential evapotranspiration, which has at least to occur since the last rewetting event to exert a maximal effect on the N_2O-production during denitrification. To describe the often observed time delay until the reaching of the maximal denitrification rate after rewetting and also to reflect the duration of the rewetting effect, an actual effective rewetting factor f_{rew} [1] is introduced:

$$f_{rew}(t) = g(t - t_j)\, f_{rew,max}(t_j) \qquad \text{for} \qquad t_j \leq t \leq t_j + 7\ , \tag{577}$$

where t_j [d] is the time of the occurrence of the rewetting event and $g(t)$ [1] is given by the following definition:

$$g(t) = \begin{cases} t/2 & \text{for } 0 \leq t \leq 2 \\ 1 & \text{for } 2 < t \leq 3 \\ 1 - (t-3)/4 & \text{for } 3 < t \leq 7 \end{cases} \tag{578}$$

The effective rewetting factor f_{rew} is then used to simulate the increased N_2O-production during denitrification after rewetting.

This is achieved by increasing the N_2O-production rate

$$k_{den,N_2O} = \; k_{den,N_2O,max} \; \tilde{e}_{\theta,d} \; \tilde{e}_{NO_3} \; e_T \; (1 + e_{thw}) \tag{579}$$

k_{den,N_2O}	N_2O production rate during denitrification $[mg\ cm^{-3}\ d^{-1}]$
$k_{den,N_2O,max}$	maximal N_2O production rate during denitrification $[mg\ cm^{-3}\ d^{-1}]$
$\tilde{e}_{\theta,d}$	modified reduction function of water content [1]
$\tilde{e}_{NO_3}$	modified reduction function of nitrate content [1]
e_T	reduction function of soil temperature [1]
e_{thw}	amplification function of thawing [1]

due to a modification of the reduction functions of water and nitrate content. For this the limiting water content value θ_d for the occurrence of denitrification is diminished by use of the effective rewetting factor f_{rew} to consider in this way the increased O_2-consumption caused by increased soil microbial activity after rewetting:

$$\tilde{\theta}_d = (1 - \alpha_\theta \; f_{rew}) \; \theta_d \qquad \text{for} \qquad \alpha_\theta = \frac{1}{3} \tag{580}$$

The insertion of the modified limiting water content $\tilde{\theta}_d$ leads to a modification of the reduction function $\tilde{e}_{\theta,d}$ of water content [1]:

$$\tilde{e}_{\theta,d} = \left[\max \left(\frac{(\theta - \tilde{\theta}_d)}{(\theta_{sat} - \tilde{\theta}_d)}, 0 \right) \right]^2 \tag{581}$$

$\tilde{e}_{\theta,d}$	modified reduction function of water content [1]
θ	vol. water content $[mm^3\ mm^{-3}]$
$\tilde{\theta}_d$	modified limiting water content for the occurrence of denitrification $[mm^3\ mm^{-3}]$
θ_{sat}	saturated vol. water content $[mm^3\ mm^{-3}]$.

Additionally, in case of rewetting the nitrate limitation of denitrification is assumed to be lowered, to simulate the higher nitrate availability in a rewetted soil. Therefore, also the reduction function of nitrate content is adapted:

$$\tilde{e}_{NO_3} = \max(e_{NO_3}, \; \alpha_{NO_3} \; f_{rew}) \qquad \text{with} \qquad \alpha_{NO_3} = 0.8 \tag{582}$$

$\tilde{e}_{NO_3}$	modified reduction function of nitrate content [1]
e_{NO_3}	original reduction function of nitrate content [1]
f_{rew}	effective rewetting factor [1] .

3.5 Mineralisation and Immobilisation

Mineralisation refers to the release of mineral carbon and nitrogen compounds during the decomposition of organic matter. Immobilisation is defined as the conversion of inorganic compounds into organic form. Both are microbial processes that are mostly in equilibrium. Immobilisation occurs when microorganisms require inorganic compounds for the synthesis of endogenous protein compounds. For example, if crop residues with a wide C/N ratio are incorporated into the soil during agricultural land use, the balance between both processes can be shifted, so that a net nitrogen immobilisation can occur for a certain time. Only when a sufficient amount of carbon from the crop residues is decomposed and partly mineralised by the soil microorganisms , i.e. partly respired to CO_2, does a net N-mineralization occur, until finally an equilibrium is restored. The nitrogen mineralised from the organic matter of the soil usually makes a considerable contribution to the nitrogen nutrition of the plant, which must be taken into account when applying fertiliser appropriate for the site.

3.5.1 Approaches of the model SOILN

The model concept of Johnsson et al. (1987) distinguishes between three different pools of organically bound N in the soil and correspondingly between three sources of available carbon for the decomposition by soil microorganisms. These three pools of organic matter consist of

- a fast decomposable organic matter pool derived from plant litter, which represents the complex of fresh organic matter and microbial biomass ('lit' for litter),
- a slowly decomposable organic matter pool, which represents the humus pool ('hum' for humus), and
- an organic matter pool, which derives from organic fertilizers mainly composed of animal faeces ('man' for manure) and which differs substantially in its chemical composition from plant residues, i.e. from the complex of fresh organic matter.

To describe the N-mineralisation and N-immobilisation of these three fractions of organic matter it is assumed, that

- the N-demand for the internal carbon cycle and humus formation is determined by a constant C/N-ratio of the decomposing microbial biomass and the newly built humus fraction, and, that
- during C-decomposition mineral N is immobilised or released by the soil microorganisms according to the actual C/N ratio of the decomposed organic matter.

3.5.1.1 C-Mineralisation The decomposition of C-compounds from fresh organic matter is caused by a reaction of first order with constant mineralisation rate k_{lit} $[d^{-1}]$, which is adapted to the actual water content and temperature of the considered soil layer by the reduction functions e_θ and e_T. We then get for the C-amount $C_{lit,dec}$ $[kg\ ha^{-1}]$, which is decomposed from fresh organic matter:

$$\frac{dC_{lit,dec}}{dt} = k_{lit}\, e_\theta\, e_T\, C_{lit} \tag{583}$$

C_{lit}	C-amount in fr. org. matter $[kg\ ha^{-1}]$	k_{lit}	mineralisation rate of fr. org. matter $[d^{-1}]$
e_θ	reduction fct. of water content [1]	e_T	reduction fct. of temperature [1]

The efficiency factor f_e [1] , which relates the C-amount newly immobilised in microbial biomass and humus to the total amount of decomposed C, determines together with the humus formation factor f_h [1] the partitioning of the decomposed C to humus, microbial biomass and CO_2 $[kg\ ha^{-1}]$ respiration:

$$\frac{dC_{lit,CO_2}}{dt} = (1 - f_e)\, \frac{dC_{lit,dec}}{dt} \tag{584}$$

$$\frac{dC_{lit,hum}}{dt} = f_e\, f_h\, \frac{dC_{lit,dec}}{dt} \tag{585}$$

$$\frac{dC_{lit,lit}}{dt} = f_e\, (1 - f_h)\, \frac{dC_{lit,dec}}{dt} \tag{586}$$

$C_{lit,dec}$	decomposed C-amount from fresh organic matter $[kg\ ha^{-1}]$		
C_{lit,CO_2}	C-amount decomposed to CO_2 from fr. org. matter $[kg\ ha^{-1}]$		
$C_{lit,hum}$	C-amount decomposed from fr. org. matter, immobilised in humus $[kg\ ha^{-1}]$		
$C_{lit,lit}$	C-amount decomposed from fr. org. matter, immobilised in microbial biomass $[kg\ ha^{-1}]$		
f_e	efficiency factor [1]	f_h	humus formation factor [1]

For the C-amount C_{lit} $[kg\ ha^{-1}]$ decomposed from fresh organic matter one gets in total:

$$\frac{dC_{lit}}{dt} = [-f_h f_e - (1 - f_e)]\frac{dC_{lit,dec}}{dt} = [-f_h f_e - (1 - f_e)]\; k_{lit}\, e_\theta\, e_T\, C_{lit} \tag{587}$$

Similarly one gets the C-amount decomposed from manure fertiliser C_{man} $[kg\ ha^{-1}]$:

$$\frac{dC_{man}}{dt} = [\,-f_h\, f_e - (1 - f_e)\,]\; k_{man}\, e_\theta\, e_T\, C_{man} \tag{588}$$

For the C-amount of humus C_{hum} $[kg\ ha^{-1}]$ one gets by additionally recognising the humus mineralisation as a first order reaction with constant reaction rate k_{hum} $[d^{-1}]$):

$$\frac{dC_{hum}}{dt} = [\, f_e\, f_h\, (k_{lit} C_{lit} + k_{man} C_{man}) - k_{hum} C_{hum}\,]\; e_\theta\, e_T \tag{589}$$

and finally for the C-amount C_{CO_2} $[kg\ ha^{-1}]$ of the mineralised, respired CO_2:

$$\frac{dC_{CO_2}}{dt} = [\ (\ 1\ -\ f_e\ )\ (\ k_{lit}C_{lit}\ +\ k_{man}C_{man}\ )\ +\ k_{hum}C_{hum}\ ]\ e_\theta\ e_T \tag{590}$$

C_{lit}	C-amount of fr. org. matter $[kg\ ha^{-1}]$	k_{lit}	mineralisation rate of fr. org. matter $[d^{-1}]$
C_{man}	C-amount of manure fertiliser $[kg\ ha^{-1}]$	k_{man}	mineralisation rate of org. man. fertiliser $[d^{-1}]$
C_{hum}	C-amount of humus $[kg\ ha^{-1}]$	k_{hum}	mineralisation rate of humus $[d^{-1}]$
e_θ	reduction fct. of water content [1]	e_T	reduction fct. of temperature [1]
f_e	efficiency factor [1]	f_h	humus formation factor [1]

3.5.1.2 N-Mineralisation The N-mineralisation resp. the N-immobilisation which occurs by the decomposition of fresh organic matter is described by:

$$\frac{dN_{lit,NH}}{dt} = (\ \frac{1}{f_{C/N,lit}}\ -\ \frac{f_e}{r_o}\ )\ \frac{dC_{lit,dec}}{dt} \tag{591}$$

$C_{lit,dec}$	C-amount decomposed from fresh organic matter $[kg\ ha^{-1}]$
$N_{lit,NH}$	N-amount of ammonium mineralised from fr. org. matter $[kg\ ha^{-1}]$
$f_{C/N,lit}$	actual C/N-ratio of fr. org. matter [1]
f_e	efficiency factor of C-decomposition [1]
r_o	C/N-ratio of decomposing microbial biomass [1]

i.e. by the difference between the N-amount decomposed to ammonium-N according to the C/N-ratio $f_{C/N,lit}$ and the N-amount fixed by the microbial biomass during decomposition. Switching between mineralisation and immobilisation occurs at a fresh organic matter C/N-ratio of r_o/f_e , i.e. if $f_{C/N,lit} = r_o/f_e$. Analogously results for the N-amount $N_{lit,hum}$ $[kg\ ha^{-1}]$ fixed by the humus pool during humus formation when fresh organic matter is decomposed:

$$\frac{dN_{lit,hum}}{dt} = \frac{f_e\ f_h}{r_o}\ \frac{dC_{lit,dec}}{dt} \tag{592}$$

For the different fractions of organic matter (lit, man, hum) then results:

$$\frac{dN_{lit}}{dt} = [\ -\frac{1}{f_{C/N,lit}}\ +\ \frac{f_e}{r_o}\ (\ 1\ -\ f_h\ )\ ]\ k_{lit}\ e_\theta\ e_T\ C_{lit} \tag{593}$$

$$\frac{dN_{man}}{dt} = [\ -\frac{1}{f_{C/N,man}}\ +\ \frac{f_e}{r_o}\ (\ 1\ -\ f_h\ )\ ]\ k_{man}\ e_\theta\ e_T\ C_{man} \tag{594}$$

$$\frac{dN_{hum}}{dt} = [\ \frac{f_e\ f_h}{r_o}\ (\ k_{lit}C_{lit}\ +\ k_{man}C_{man}) - k_{hum}N_{hum}\ ]\ e_\theta\ e_T \tag{595}$$

N_{lit}	N-amount of fr. org. matter $[kg\ ha^{-1}]$	N_{man}	N-amount of manure fertiliser $[kg\ ha^{-1}]$
N_{hum}	N-amount of humus $[kg\ ha^{-1}]$	k_{hum}	mineralisation rate of humus $[d^{-1}]$
C_{lit}	C-amount of fr. org. matter $[kg\ ha^{-1}]$	k_{lit}	mineralisation rate of fr. org. matter $[d^{-1}]$
C_{man}	C-amount of manure fertiliser $[kg\ ha^{-1}]$	k_{man}	mineralisation rate of manure fertiliser $[d^{-1}]$
e_θ	reduction fct. of water content [1]	e_T	reduction fct. of temperature [1]
f_e	efficiency factor [1]	f_h	humus formation factor [1]
r_o	C/N-ratio of the decomposing microbial biomass [1]		
$f_{C/N,x}$	C/N-ratio [1] of fresh organic matter resp. manure fertiliser $(x = lit, man)$		

and finally result the sink resp. source terms of the solute transport equations, see (420), per numerical layer, if divided by the layer thickness of the respective layer $\Delta z\ [mm]$ to convert from amounts $\Phi_I\ [kg\ ha^{-1}]$ to concentrations $S_{c,I}\ [mg\ dm^{-3}]$, i.e. $S_{c,I} = \Phi_I / \Delta z$:

$$\begin{aligned}\Phi_{Min} \;=\; \{\, & k_{hum} N_{hum} \;+\; \max[\,0,0;(\,\frac{1}{f_{C/N,lit}} \;-\; \frac{f_e}{r_o}\,)\,]\; k_{lit} C_{lit} \\ & +\; \max[\,0,0;(\,\frac{1}{f_{C/N,man}} \;-\; \frac{f_e}{r_o}\,)\,]\; k_{man} C_{man}\,\}\; e_\theta\; e_T \end{aligned} \tag{596}$$

$$\begin{aligned}\Phi_{Imm,NH} \;=\; \{\, & \min[\,0,0;(\,\frac{1}{f_{C/N,lit}} \;-\; \frac{f_e}{r_o}\,)\,]\; k_{lit} C_{lit} \\ & +\; \min[\,0,0;(\,\frac{1}{f_{C/N,man}} \;-\; \frac{f_e}{r_o})]\; k_{man} C_{man}\,\}\; r_{NH}\; e_\theta\; e_T \end{aligned} \tag{597}$$

$$\Phi_{Imm,NO} \;=\; \Phi_{Imm,NH}\, \frac{r_{NO}}{r_{NH}} \tag{598}$$

where

$$r_{NH} = \frac{(\,\theta \;+\; \rho_s K_{d,NH})\, c_{NH}}{(\,\theta \;+\; \rho_s K_{d,NH})\, c_{NH} \;+\; \theta\, c_{NO}}, \qquad r_{NO} = 1 - r_{NH}$$

Φ_{Min}	ammonium-N source by mineralisation $[kg\ ha^{-1}\ d^{-1}]$
$\Phi_{Imm,NH}$	ammonium-N sink by immobilisation $[kg\ ha^{-1}\ d^{-1}]$
$\Phi_{Imm,NO}$	nitrate sink by immobilisation $[kg\ ha^{-1}\ d^{-1}]$
r_{NH}	ratio of ammonium-N to ammonium- and nitrate-N [1]
r_{NO}	ratio of nitrate-N to ammonium- and nitrate-N [1]
θ	volumetric water content $[mm^3\ mm^{-3}]$
ρ_s	soil bulk density $[kg\ dm^{-3}]$
$K_{d,NH}$	adsorption coefficient of ammonium-N $[dm^3\ kg^{-1}]$
c_{NH}	ammonium-N concentration in soil solution $[mg\ dm^{-3}]$
c_{NO}	nitrate-N concentration in soil solution $[mg\ dm^{-3}]$

3.5.2 Approaches of the Model CERES-N

The approach chosen in the models CERES and N-SIM to describe mineralisation and immobilisation is based on the PAPRAN model. (Seligman and van Keulen, 1981). It is an attempt to simulate the functionality of models describing the processes at the microorganism level with very simple approaches. Mineralisation and immobilisation of Nitrogen are modeled by the degradation of organic matter using first order reaction rates. The model distinguishes between fresh organic matter (FOM), composed of harvest residues and green manure, and a pool of more stable organic matter, the humus pool (HUM).

3.5.2.1 C-Mineralisation The pool of FOM $[kg\ ha^{-1}]$ is further divided into the fractions carbohydrates, cellulose and lignin. The decomposition rates of these FOM-fractions $k_I\ [d^{-1}]$ with index $I = CH$ for carbohydrate, $I = CL$ for cellulose und $I = LI$ for Lignin are defined by the maximal decomposition rates $k_{I,max}\ [d^{-1}]$ and by the following equations:

$$k_I = k_{I,max}\ f_\theta\ f_T\ f_{C/N} \tag{599}$$

f_θ	reduction fct. of water content $[1]$
f_T	reduction fct. of temperature $[1]$
$f_{C/N}$	reduction factor due to N-limitation during decomposition of FOM $[1]$
$k_{I,max}$	maximal decomposition rates $[d^{-1}]$ of FOM (carbohydrates CH, cellulose CL, lignin LI)

The maximal decomposition rates $k_{I,max}\ [d^{-1}]$, which are applied for FOM decomposition under optimal, nonlimiting conditions, are given by $k_{CH,max} = 0,2\ d^{-1}$, $k_{CL,max} = 0,05\ d^{-1}$ und $k_{LI,max} = 0,0095\ d^{-1}$. This means for the decomposition of carbohydrates, that under favourable conditions 20% of this fraction are decomposed within one day.
The water content function f_θ [1] considers the impact of soil moisture on the mineralisation.

$$f_\theta = \begin{cases} (\theta - 0,5\ \theta_{pwp})/(\theta_{fc} - 0,5\ \theta_{pwp}) & \text{for } \theta \leq \theta_{fc} \\ 1,0 - 0,5\ (\theta - \theta_{fc})/(\theta_{max} - \theta_{fc}) & \text{for } \theta > \theta_{fc} \end{cases} \tag{600}$$

f_θ	reduction fct. of water content $[1]$
θ	act. vol. water content $[mm^3\ mm^{-3}]$
θ_{pwp}	vol. water content at permanent Wilting point $[mm^3\ mm^{-3}]$
θ_{fc}	vol. water content at fieldcapacity $[mm^3\ mm^{-3}]$
θ_{max}	maximal vol. water content $[mm^3\ mm^{-3}]$, see eq.. (226)

According to Myers et al. (1982) and Linn und Doran (1984) optimal conditions of mineralisations are given at water content within the range of fieldcapacity. With decreasing water contents the mineralisation will be restricted, but only comes to a standstill when the soil is air dry (50% of the water content at permanent wilting point). Under very wet conditions, only half as much is mineralised as under optimal conditions.
The temperature function f_T $[1]$, which considers the impact of soil temperature T of the respective soil layer on the mineralisation within this layer, is given by:

$$f_T = \begin{cases} 0,0 & \text{for } T < 0,0°C \\ T/30°C & \text{for } 0,0°C \leq T \leq 30°C \\ 1,0 & \text{for } T > 30°C \end{cases} \tag{601}$$

The third reduction factor $f_{C/N}$ $[1]$, which indicates the possible inhibition of mineralisation by the C/N ratio of the crop residues inorporated into the soil, is calculated according to the following formula

$$f_{C/N} = \exp\{-0,693\ [C_{FOM}/(N_{FOM}\ +\ N_{min}) - 25,0]/25,0\} \tag{602}$$

where the C/N ratio establishing in the soil is derived from the carbon contained in the fresh organic matter C_{FOM} $[kg\ ha^{-1}]$ (40% C fraction of total FOM) and the nitrogen available for the decomposition process (N in fresh organic matter N_{FOM} $[kg\ ha^{-1}]$ and mineral nitrogen N_{min} $[kg\ ha^{-1}]$).

3.5.2.2 N-Mineralisation The Nitrogen $N_{FOM,min}$ $[kg\ ha^{-1}]$ mineralised from the fractions of fresh organic matter(FOM) having a dry weight W_{FOM} $[kg\ ha^{-1}]$ per time step and soil layer is the sum of the respective proportions of the fractions f_I $[1]$ in the total amount of FOM, the respective mineralisation rates k_I $[d^{-1}]$ and the nitrogen amount N_{FOM} $[kg\ ha^{-1}]$ of FOM:

$$\frac{d\,W_{FOM,min}}{dt} = (k_{KH}\,f_{KH} + k_{ZL}\,f_{ZL} + k_{LI}\,f_{LI})\,FOM \tag{603}$$

$$\frac{d\,N_{FOM,min}}{dt} = \frac{N_{FOM}}{W_{FOM}}\,\frac{d\,W_{FOM,min}}{dt} \tag{604}$$

When FOM is decomposed, the soil microorganisms themselves need nitrogen to build up their own biomass, i.e. a certain proportion of the FOM nitrogen $N_{FOM,imm}[kg\ ha^{-1}]$ is immobilised during the mineralisation process . This N portion is calculated from the portion which cannot be covered by the N from the FOM, i.e. which cannot be mineralised and is therefore withdrawn from the soil pool of mineral N:

$$\frac{d\,N_{FOM,imm}}{dt} = 0,02\ \min(\frac{d\,W_{FOM,min}}{dt};\frac{N_{min}}{1,0d}) \tag{605}$$

Thereby it is assumed that the N-demand of the microbial biomass accounts for 2% of the total FOM during FOM decomposition. This value of 2% results from the C component of the FOM (=40%), the biological effectiveness of the microbial C decomposition (= 0.4) and the reciprocal of the C/N-ratio of the soil microorganisms (= 0.125).

The net N-Mineralisierung from FOM finally results from:

$$\frac{d\,N_{FOM}}{dt} = \frac{d\,N_{FOM,imm}}{dt} - \frac{d\,N_{FOM,min}}{dt} \tag{606}$$

and the decomposition of total FOM from:

$$\frac{d\,W_{FOM}}{dt} = -\frac{d\,W_{FOM,min}}{dt} \tag{607}$$

In a similar way as the decomposition of FOM, the decomposition of the more stable organic matter, the humus fraction (HUM) is modeled. The N-release from the organic nitrogen N_{HUM} $[kg\ ha^{-1}]$ bound in the humus pool occurs with a very small decomposition rate of first order $k_{HUM} = 0.83\ 10^{-4} d^{-1}$ under consideration of the humidity and temperature functions as used in describing the FOM decomposition:

$$\frac{d\,N_{HUM,min}}{dt} = k_{HUM}\ f_\theta\ f_T\ N_{HUM} \tag{608}$$

For the decomposition of humus dry matter W_{HUM} $[kg\ ha^{-1}]$ and the nitrogen in humus N_{HUM} $[kg\ ha^{-1}]$ it is assumed, that 20% of the nitrogen released from fresh organic matter (FOM) is determined in the form of N compounds, that are difficult to degrade and thus are attributable to the humus fraction. Further, a N-content of 4% is assumed for the forming humus (C-content:40%, C/N-ratio: 10,0):

$$\frac{d\,N_{HUM}}{dt} = -\frac{d\,N_{HUM,min}}{dt} + 0,2\,\frac{d\,N_{FOM,min}}{dt} \tag{609}$$

$$\frac{d\,W_{HUM}}{dt} = \frac{1}{0,04}\,\frac{d\,N_{HUM}}{dt} \tag{610}$$

In total, a sink term by mineralisation is obtained for the organic bound nitrogen and thus a source term for the ammonium nitrogen Φ_{Min} $[kg\ ha^{-1}\ d^{-1}]$

$$\Phi_{Min} = \frac{d\,N_{FOM,min}}{dt} + \frac{d\,N_{HUM,min}}{dt} \tag{611}$$

and also a sink term for ammonium-N by immobilisation $\Phi_{Imm,NH}$ $[kg\ ha^{-1}\ d^{-1}]$

$$\Phi_{Imm,NH} = 0,2\,\frac{d\,N_{FOM,min}}{dt} + \frac{d\,N_{FOM,imm}}{dt} \tag{612}$$

3.5.3 Approach of the model DAISY

The model for the turnover of the organic matter, which is used in the model DAISY (Svendsen et al., 1995), distinguishes three soil organic matter pools: the fresh organic matter AOM supplied (added organic matter), the microbial biomass SMB (soil microbial biomass) and the dead, soil-borne organic matter SOM (soil organic matter). Each of these pools of organic matter is divided into two sub-pools, which are each further subdivided by assignment of a different constant carbon-nitrogen ratio and a different decomposition rate.
Thus, the supply of soil-borne organic substance SOM is divided into the sub-pools SOM1 and SOM2. SOM1 is the more chemically stabilized organic matter consisting of organic compounds that are biologically difficult to decompose. SOM2 consists of the more physically stabilized organic matter, which is protected against biological decomposition by adsorption to soil colloids or by inclusion into soil aggregates.

3.5.3.1 C-Mineralisation The decomposition rates of SOM1 and SOM2 are impacted by the soil temperature T $[°C]$, by the soil water content represented as soil matric potential h $[kPa]$ and by the clay content $[\%]$. The rates are described by first order reaction kinetics with rate constants k_{SOMi} $[d^{-1}]$ and reduction functions of temperature g_T $[1]$, of soil water content g_h $[1]$ and of clay content g_{clay} $[1]$ using

$$\frac{dC_{SOMi,dec}}{dt} = k_{SOMi}\, g_T\, g_h\, g_{clay}\, C_{SOMi}, \quad i = 1, 2 \tag{613}$$

and the following abbreviations:

$dC_{SOMi,dec}/dt$	carbon decomposition rate of $SOMi$ $[kg\ ha^{-1}d^{-1}]$
C_{SOMi}	carbon amount of pool $SOMi$ in the soil layer i $[kg\ ha^{-1}]$
g_T	reduction function of soil temperature [1]
g_h	reduction function of soil water content [1] as function of soil the matric potential h
g_{clay}	reduction function of clay content [1]
k_{SOMi}	rate constant of the first order rate of $SOMi$-decomposition $[d^{-1}]$

The abiotic reduction functions adapt the decomposition rates of organic matter, as they occur under standard conditions, to the actual states of soil temperature, soil water and clay content. The reduction function of clay content expresses the stronger physical and chemical protection of more clayey soils against biological decomposition.

The function g_{clay} $[1]$ is defined by:

$$g_{clay}(x) = \begin{cases} 1 \,-\, 2\,x & 0 \,<\, x \,\leq\, x_l \\ 1 \,-\, 2\,x_l & x \,>\, x_l \end{cases} \tag{614}$$

$g_{clay}(x)$	reduction function of clay content [1]
x	clay content $[kg\ kg^{-1}]$
x_l	limit value of the higher protection against decomposition by clay content (= 0,25 $[kg\ kg^{-1}]$

The turnover rates of soil organic matter are significantly influenced by soil temperature. Although little is known about the turnover at temperatures below 5°C, it is assumed that the rates near 0°C tend to zero. Furthermore, it is assumed that the effect of soil temperature increases linearly between 0-20°C and exponentially with temperature in the range above 20°C:

$$g_T(T) = \begin{cases} 0 & T \,\leq\, 0°C \\ 0,1\,T & 0 \,<\, T \,\leq\, 20°C \\ \exp(0,47 - 0,027T + 0,00193T^2) & T \,>\, 20°C \end{cases} \tag{615}$$

$g_T(T)$	impact function of soil temperature [1]
T	soil temperature [°C]

To model the reduction function of water content it is assumed, that the turnover rate of soil organic matter at a soil matric potential of pF=6.5 is almost zero and, that in the range of 1.5 < pF < 2.5 the turnover is optimal. Furthermore, it is assumed, that the function increases linearly from a value of 0.6 at soil water saturation to 1.0 at pF = 1.5 and, that it linearly decreases from 1.0 at pF = 2.5 to 0.0 at pF = 6.5:

$$g_h(h) = \begin{cases} 0.6 & h \,\geq\, -(10^{-2}) \\ 0.6 \,+\, 0.4\,log(-100h)/1.5 & -(10^{-2} \,>\, h \,\geq\, -(10^{-0.5}) \\ 1.0 & -(10^{-0.5}) \,>\, h \,\geq\, -(10^{0.5}) \\ 1.0 \,-\, log(-100h)/4.0 & -(10^{0.5} \,>\, h \,\geq\, -(10^{4.5}) \\ 0 & -(10^{4.5}) \,>\, h \end{cases} \tag{616}$$

$g_h(h)$	reduction function of soil water content [1]
h	soil matric potential $[m]$ (water column)

Although the soil microbial biomass SMB usually accounts for only about three percent of the organic bound carbon in soil, it is of great importance for the total soil C and N turnover due to the production of exoenzymes and the turnover of organic matter dissolved in soil water. In order to be able to describe a relatively stable, but also dynamic pool of microbial biomass, a distinction is made between a stable fraction SMB1 and a dynamic fraction

SMB2 of soil microbial biomass. The two components are characterized by different mortality rates and different consumption of dissolved organic matter as substrate and energy source.

For the microbial biomass pools SMB1 and SMB2, i.e. for the carbon pools C_{SMBi} $[kg\ ha^{-1}]$ in the respective soil layer, the death and decomposition rates are again described by first order rates and correspondingly given by maximal specific death rates d_{SMBi} $[d^{-1}]$ and specific maintenance coefficients m_{SMBi} $[d^{-1}]$. With reduction functions of temperature g_T [1], water content g_h [1] and clay fraction g_{clay} [1] result the decomposition rates of microbial biomass carbon $C_{SMBi,dec}$ $[kg\ ha^{-1}]$ $i = 1, 2$:

$$\frac{dC_{SMB1,dec}}{dt} = (d_{SMB1} + m_{SMB1}) \, g_T \, g_h \, g_{clay} \, C_{SMB1} \tag{617}$$

$$\frac{dC_{SMB2,dec}}{dt} = (d_{SMB2} + m_{SMB2}) \, g_T \, g_h \, C_{SMB2} \tag{618}$$

and the death rates

$$\frac{dC_{SMB1,d}}{dt} = d_{SMB1} \; g_T \, g_h \, g_{clay} \, C_{SMB1} \tag{619}$$

$$\frac{dC_{SMB2,d}}{dt} = d_{SMB2} \; g_T \, g_h \, C_{SMB2} \tag{620}$$

The added organic matter AOM can consist of stall manure or dung , slurry, green manure and of plant residues left on the field after harvest. It is partitioned to the pools AOM1, AOM2 and SOM2 corresponding to the quality of the characteristic fractions f_{AOM1} [1], f_{AOM2} [1], and $1 - f_{AOM1} - f_{AOM2}$ [1] of the AOM. Thereby, AOM1 denotes the added organic matter, which is more difficult to decompose and mainly consists of material from cell walls.

AOM2 characterizes added, more easily decomposable matter, which is mainly composed by water extractable cell compounds. For organic fertilizers, as for example for stall manure, for which partly already decomposition processes took place, a certain part of organic matter is finally allocated to the SOM2 pool, which consists of lignin and other compounds resistant to microbial degradation.

The decomposition rates $dC_{AOMi,dec}/dt$ $[kg\ ha^{-1}d^{-1}]$ of carbon C_{AOMi} $[kg\ ha^{-1}]$ of AOM1 resp. AOM2 are again given by raction kinetics of first order having rate constants k_{AOMi} $[d^{-1}]$ and reduction functions:

$$\frac{dC_{AOMi,dec}}{dt} = k_{AOMi} \, g_T \, g_h \, C_{AOMi}, \; i = 1, 2 \tag{621}$$

The addition of organic matter AOM is modeled by a Dirac-pulse function, such that the addition occurs within a time step in between the time steps t_0 and $t_0 + \Delta t$:

$$I_\Delta = \begin{cases} \frac{I_{AOM}}{\Delta t}, \ t_0 \ \leq \ t \ < \ t_0 + \Delta t \\ 0, \ sonst \end{cases} \tag{622}$$

I_Δ	input function $[kg \ ha^{-1} \ d^{-1}]$ per soil layer
I_{AOM}	input of organic matter $[kg \ ha^{-1}]$ per soil layer
t	time [d]
Δt	time step between consecutive time points of the simulation

The carbon balance of organic matter in the soil and its turnover within the six different soil organic matter pools AOM1, AOM2, SMB1, SMB2, SOM1 and SOM2 is described per soil layer by the following six equations:

The change of the pools AOM1 and AOM2 is balanced from the input of organic matter AOM, which is partitioned by means of the partition factors $f_{AOM1}[1]$ and $f_{AOM2}[1]$, and by the respective decomposition rates $dC_{AOMi,dec}/dt \ [kg \ ha^{-1}d^{-1}]$ of the pools:

$$\frac{dC_{AOM1}}{dt} = f_{AOM1} \, I_\Delta \ - \ \frac{dC_{AOM1,dec}}{dt} = f_{AOM1} \, I_\Delta \ - \ k_{AOM1} \, g_T \, g_h \, C_{AOM1} \tag{623}$$

$$\frac{dC_{AOM2}}{dt} = f_{AOM2} \, I_\Delta \ - \ \frac{dC_{AOM2,dec}}{dt} = f_{AOM2} \, I_\Delta \ - \ k_{AOM2} \, g_T \, g_h \, C_{AOM2} \tag{624}$$

The development of the stable microbial biomass pool is calculated by considering the carbon loss by death and the carbon yield by the microbial biomass

- from the decomposition of the more stable pool $dC_{SOM1,dec}/dt \ [kg \ ha^{-1}d^{-1}]$ of soil borne organic matter,
- from the fraction of the decomposition $(1 - f_{SOM1}) \ dC_{SOM2,dec}/dt \ [kg \ ha^{-1}d^{-1}]$ of the more labile pool, which is not allocated to the stable pool SOM1 and is given by the partition factor $(1 - f_{SOM1})$ [1],
- from the decomposition of the more stable pool $f_{SMB1} \ dC_{AOM1,dec}/dt$ of added organic matter with partition factor f_{SMB1} [1]
- and the carbon consumption for maintenance respiration:

$$\frac{dC_{SMB1}}{dt} = e_{SMB1} \, [\, \frac{dC_{SOM1,dec}}{dt} \ + \ (1 - f_{SOM1}) \, \frac{dC_{SOM2,dec}}{dt} + \tag{625}$$

$$+ \, f_{SMB1} \, \frac{dC_{AOM1,dec}}{dt} \,] \ - \ \frac{dC_{SMB1,dec}}{dt}$$

For the more dynamic and more labile pool of microbial biomass carbon results the carbon balance

- by the substrate consumption rate of available dead microbial biomass, which does not belong to the pool SOM2 gehört: $(1 - f_{SOM2})\ (dC_{SMB1,d}/dt\ +\ dC_{SMB2,d}/dt)$ $[kg\ ha^{-1} d^{-1}]$,
- by the decomposition rate of the stable pool of added organic matter, which can be faster consumed and is not used by the pool SMB1 $(1\ -\ f_{SMB1})\ dC_{AOM1,dec}/dt$ $[kg\ ha^{-1} d^{-1}]$ with partition factor $(1 - f_{SMB1})$ [1],
- by the decomposition rate of the labile pool of added organic matter $dC_{AOM2,dec}/dt$ $[kg\ ha^{-1} d^{-1}]$
- and by the decomposition rate of the microbial carbon pool $dC_{SMB2,dec}/dt$ $[kg\ ha^{-1} d^{-1}]$ given by maintenance metabolism and death:

$$\frac{dC_{SMB2}}{dt} = e_{SMB2}\,[\,(1 - f_{SOM2})\,(\,\frac{dC_{SMB1,d}}{dt} + \frac{dC_{SMB2,d}}{dt}\,) + \tag{626}$$

$$+\,(1 - f_{SMB1})\,\frac{dC_{AOM1,dec}}{dt} + \frac{dC_{AOM2,dec}}{dt}\,] - \frac{dC_{SMB2,dec}}{dt}$$

The change of both pools of organic matter, the SOM1 and the SOM2 pool, is calculated by considering

- the respective decomposition rates $dC_{SOM1,dec}/dt$ and $dC_{SOM2,dec}/dt$ of the pools
- the fraction of decomposed, more labile SOM2 pool $f_{SOM1}\ dC_{SOM2,dec}/dt$, which reaches by decomposition a more stable state, and gets part of the SOM1 pool
- the fraction of dead microbial biomass $f_{SOM2}(dC_{SMB1,d}/dt{+}dC_{SMB2,d}/dt)$, which is not immediately used by microorganism as a substrate, but added to the more labile pool of organic mattter SOM2
- the fraction of added organic matter $(1 - f_{AOM1} - f_{AOM2})\ I_{\Delta}$ added to the more labile pool SOM2 :

$$\frac{dC_{SOM1}}{dt} = f_{SOM1}\,\frac{dC_{SOM2,dec}}{dt} - \frac{dC_{SOM1,dec}}{dt} \tag{627}$$

$$\frac{dC_{SOM2}}{dt} = (1 - f_{AOM1} - f_{AOM2})\,I_{\Delta} + f_{SOM2}\,(\frac{dC_{SMB1,d}}{dt} + \frac{dC_{SMB2,d}}{dt}) - \frac{dC_{SOM2,dec}}{dt} \tag{628}$$

The CO_2 respiration of the soil microorganisms finally results by applying the efficiency factors e_{SMB1} [1] and e_{SMB2} [1] and from the maintenance respiration:

$$\frac{dC_{CO_2}}{dt} = (1 - e_{SMB1})[\frac{dC_{SOM1,dec}}{dt} + (1 - f_{SOM1})\frac{dC_{SOM2,dec}}{dt} + f_{SMB1}\frac{dC_{AOM1,dec}}{dt}] + (1 - e_{SMB2})[(1 - f_{SOM2})(\frac{dC_{SMB1,d}}{dt} + \frac{dC_{SMB2,d}}{dt}) + (1 - f_{SMB1})\frac{dC_{AOM1,dec}}{dt}] + (1 - e_{SMB2})\frac{dC_{AOM2,dec}}{dt} + (\frac{dC_{SMB1,dec}}{dt} - \frac{dC_{SMB1,d}}{dt}) + (\frac{dC_{SMB2,dec}}{dt} - \frac{dC_{SMB2,d}}{dt}) \tag{629}$$

3.5.3.2 N-Mineralisation To calculate the C- and N-mineralisation-immobilisation-turnover by the model concept of the model DAISY it is assumed, that the net N-mineralisation can be determined mainly by

- the rates, by which the organic matter is dissolved in soil solution to build substrate for the soil microorganisms
- the efficiency by which the soil microorganisms use dissolved organic matter
- the C/N-ratios $f_{C/N,x}$ [1] assumed to be different constants for the differentpools of organic matter ($x = AOMi, SOMi$), which are decomposed and
- the C/N-ratios $f_{C/N,SMBi}$ [1] also assumed to be different constants for the different pools of microorganisms $SMBi$ $[kg\ ha^{-1}]$

By this, the net N-mineralisation is mainly dependent on the N-storage in the soil organic matter pools, the quality of these pools and their fixed C/N-ratios.

From the C-balance of each single pool of organic matter and by the fixed C/N-ratios results a total balance of the nitrogen bound to organic matter, which leads to an equation of the N-mineralisation-immobilisation-turnover Φ_{NMIT} $[kg\ ha^{-1}\ d^{-1}]$, of the net N-mineralisation Φ_{Min} $[kg\ ha^{-1}\ d^{-1}]$ and the net N-Immobilisation Φ_{Imm} $[kg\ ha^{-1}\ d^{-1}]$:

$$\begin{aligned}
\Phi_{NMIT} \quad = \quad & f^{-1}_{C/N,AOM1}\,\frac{dC_{AOM1,dec}}{dt} \;+\; f^{-1}_{C/N,AOM2}\,\frac{dC_{AOM2,dec}}{dt} \\
& + f^{-1}_{C/N,SOM1}\,\frac{dC_{SOM1,dec}}{dt} \;+\; f^{-1}_{C/N,SOM2}\,\frac{dC_{SOM2,dec}}{dt} \\
& - f_{SOM1}\, f^{-1}_{C/N,SOM2}\,\frac{dC_{SOM2,dec}}{dt} \\
& - f_{SOM2}\,(f^{-1}_{C/N,SMB1}\,\frac{dC_{SMB1,d}}{dt} \;+\; f^{-1}_{C/N,SMB2}\,\frac{dC_{SMB2,d}}{dt}) \\
& - f^{-1}_{C/N,SMB1}\,\frac{dC_{SMB1}}{dt} \;-\; f^{-1}_{C/N,SMB2}\,\frac{dC_{SMB2}}{dt}
\end{aligned} \tag{630}$$

$$\Phi_{Min} \quad = \quad \max\{0;\Phi_{NMIT}\} \tag{631}$$

If the N-turnover Φ_{NMIT} gets negative, i.e. if a net N-immobilisation takes place, this will be limited by maximal specific immobilisation rates $k^{imm}_{NH,max}$ $[d^{-1}]$ for ammonium-N resp. $k^{imm}_{NO,max}$ $[d^{-1}]$ for nitrate-N, by which the soil microorganisms can provide themselves by the mineral soil N-pool $N_{NH} + N_{NO}$ $[kg\ ha^{-1}]$:

$$\Phi_{Imm,NH} \quad = \quad -\ \min\{0;\max\{\Phi_{NMIT};-\,k^{imm}_{NH,max}\,N_{NH}\}\} \tag{632}$$

$$\Phi_{Imm,NO} \quad = \quad -\ \min\{0;\max\{\Phi_{NMIT};-\,k^{imm}_{NO,max}\,N_{NO}\}\} \tag{633}$$

$$\Phi_{Imm} \quad = \quad \Phi_{ImmNH} \;+\; \Phi_{ImmNO} \tag{634}$$

3.5.4 Approaches of the model EXPERT-N

Further mineralisation models were implemented into the EXPERT-N model system. These are the corresponding sub-models of NCSOIL (Molina et al., 1983), DNDC (Li et al., 1992) and NITS (Birkenshaw and Ewen, 2000). In addition, a modified version of the CERES approach has been developed which, like the other models, considers C turnover instead of dry matter turnover in the soil pools of fresh organic matter and humus and also describes the resulting CO_2 release. Also EXPERT-N own model variants for C- and N-mineralisation were integrated, which are based on the models SOILN resp. NITS and additionally model the pool of soil microorganisms involved in the turnover. In addition, a model was developed to simulate the decomposition and mineralisation of organic matter standing or lying on the surface of arable soils (Berkenkamp et al., 2002). This model also serves as a general surface mineralisation model, which can partition the given input of soil organic matter supply to the corresponding soil pools of the selected mineralisation model.

3.5.4.1 Organic Matter Turnover at the Soil Surface The model for the description of turnover and decomposition of organic matter on the soil surface combines (i) the differentiation of three pools of organic matter as conceived by the model SOILN (Johnsson et al., 1987) with (ii) the division of aboveground organic substances into horizontal and vertical components as given by the model RESMAN (Stott et al., 1995) and (iii) the description of the incorporation of organic matter into the soil as applied by the model EPIC (Grant et al., 1998). Therefore, three surface pools of organic matter are introduced into the model, the surface pool of plant residues, the surface pool of organic fertilizer from animal faeces and the surface pool of humus. These three soil surface pools represent the organic matter on the soil surface that is subject to mineralisation. In addition, the reservoir of standing dead plant biomass is taken into account, which is gradually reduced by weathering impacts or cultivation measures, and is thus adding to the surface pool of lying plant residues. In contrast to the SOILN model approach for the soil litter pool, the surface pool of plant residues also includes the total microbial biomass that causes the degradation of organic matter on the soil surface. In addition to these pools of organic matter, also the mineral nitrogen enriched on the soil surface by manure or mineralisation is described, which provides the N-source for the N-immobilisation during the degradation of the surface pools in form of ammonium-N or nitrate-N .

Organic matter, that is deposited at the soil surface is partitioned to the corresponding surface pools according to its origin: Crop residues after harvest to the surface pool of standing or lying plant residues, organic fertilizers to the pool of organic matter from animal faeces and finally more difficult to decompose organic material resp. already largely decomposed organic matter to the humus surface pool. The partitioning of plant residues into standing or lying fractions is achieved by applying a cutting factor, f_{ha} [1], which represents the ratio of the mean crop cutting height of harvest h_{cut} $[m]$ to the maximal crop height h_{max} $[m]$:

$$f_{ha} \;=\; h_{cut}/h_{max} \tag{635}$$

By this, the input functions into the surface pools of standing plant residues $I_{ha,st}$ $[kg\ ha^{-1}\ d^{-1}]$ resp. of lying plant residues $I_{ha,ls}$ $[kg\ ha^{-1}\ d^{-1}]$ at time t_0 $[d]$ of harvest can be defined:

$$I_{ha,st} \;=\; \begin{cases} \dfrac{f_{ha}C_{res}}{\Delta t}, & t_0 \;\leq\; t \;<\; t_0+\Delta t \\ 0\;, & \text{sonst} \end{cases} \tag{636}$$

$$I_{ha,ls} \;=\; \begin{cases} \dfrac{(1-f_{ha})C_{res}}{\Delta t}, & t_0 \;\leq\; t \;<\; t_0+\Delta t \\ 0\;, & \text{sonst} \end{cases} \tag{637}$$

$I_{ha,st}$	Input function of the standing pool of organic matter $[kg\ ha^{-1}\ d^{-1}]$
$I_{ha,ls}$	Input function of the lying Pool of organic matter $[kg\ ha^{-1}\ d^{-1}]$
Δt	time step between two consecutive times of the simulation [d]
f_{ha}	cutting factor[1]
C_{res}	carbon content of plant residues $[kg\ ha^{-1}]$

If a catch crop dies due to frost, its total organic matter is added to the surface pool of standing plant residues. Since during strong wind or heavy precipitation parts of the dead plants fall to the soil, it is assumed according to Stott et al. (1995), that per day 1% of the C- and N-amounts of the standing surface pool are transferred to the lying surface pool of plant residues.

The decrease of C-amounts of the standing surface pool by soil cultivation is modeled by an approach of the EPIC-model (Williams et al., 1989), i.e. by defining a transfer function or incorporation function $T_{st,ls}$ $[kg\ ha^{-1}\ d^{-1}]$:

$$T_{st,ls} \;=\; \begin{cases} -\,\dfrac{C_{st}}{\Delta t}\,[1-\exp(-56,9\;z_{til}\;I_f^2)], & t_0 \;\leq\; t \;<\; t_0+\Delta t \\ 0\;, & \text{sonst} \end{cases} \tag{638}$$

Δt	time step between two consecutive times of simulation [d]		
C_{st}	C-content of the standing surface pool $[kg\ ha^{-1}]$	z_{til}	soil cultivation depth $[mm]$
t	time [d]	t_0	time of soil cultivation [d]
I_f	efficiency of incorporation in dependence of the kind of soil cultivation [1]		

Similar equations describe the decrease of organic matter surface pools during soil cultivation by defining transfer functions $T_{ms,man}$ $[kg\ ha^{-1}\ d^{-1}]$ and $T_{hs,hum}$ $[kg\ ha^{-1}\ d^{-1}]$ to the corresponding pools of organic matter (of organic fertilizer or humus), where in case of the transfer function $T_{ls,lit}$ $[kg\ ha^{-1}\ d^{-1}]$ to the pool of lying plant residues it is assumed, that a part of the organic matter, which was transferred from the standing pool into the lying pool, is further incorporated by the same soil cultivation into the top soil:

$$T_{ls,lit} = \begin{cases} -\dfrac{(C_{ls} + T_{st,ls})}{\Delta t}\,[1 - \exp(-56,9\ z_{til}\ I_f^2)], & t_0 \le t < t_0 + \Delta t \\ 0\quad , & \text{sonst} \end{cases} \tag{639}$$

Δt	time step between two consecutive times of simulation [d]		
C_{ls}	C-content of the lying surface pool $[kg\ ha^{-1}]$	z_{til}	soil cultivation depth $[mm]$
t	time [d]	t_0	time of soil cultivation [d]
I_f	efficiency of incorporation in dependence of the kind of soil cultivation [1]		

The increase of the below-ground pools by the incorporation of organic matter occurs in combination with a homogenisation of these pools within the incorporation depth. First, the part of the organic matter that is subtracted from the surface pools is added to the corresponding soil organic matter pools in the first numerical layer. Then corresponding organic matter pools of all numerical layers within the incorporation depth are each homogeneously mixed and uniformly distributed to all numerical layers within this depth. This homogenisation within the soil cultivation depth will be calculated using the transfer function $T_{til,x}$ $[kg\ ha^{-1}\ d^{-1}]$ for mixing the soil organic matter pool x during tillage (Williams et al., 1989), where $x = lit$ stands for the soil organic matter from plant residues, $x = man$ for those from organic fertilizers and $x = hum$ for the humus pool:

$$T_{til,x} = \begin{cases} 1 - I_f\,\dfrac{C_{x,i}}{\Delta t} + \dfrac{\Delta z_i}{z_{til}}\,I_f \displaystyle\sum_{i=1}^{m} \dfrac{C_{x,i}}{\Delta t}, & \text{for}\quad t_0 \le t < t_0 + \Delta t \\ 0\quad , & \text{sonst} \end{cases} \tag{640}$$

$C_{x,i}$	C-amount of soil organic matter pool x $(= lit, man, hum)$ $[kg\ ha^{-1}]$		
Δt	time step between two consecutive times of simulation [d]		
I_f	efficiency of incorporation in dependence of the kind of soil cultivation [1]		
m	number of numerical soil layers within the incorporation depth [1]		
z_{til}	incorporation depth $[mm]$	Δz_i	thickness of the i-th soil layer $[mm]$
t	time [d]	t_0	time of soil cultivation [d]

The C-amounts and corresponding N-amounts of the considered soil surface resp. soil pools of organic matter are calculated using the C/N-ratios of these pools.

3.5.4.2 C-Mineralisation at the Soil Surface The decomposition of the organic matter in the three above-ground pools subject to mineralisation is modeled according to the SOILN model, each with a reaction kinetics of first order including the temperature function and reduction function of soil water content (Berkenkamp et al., 2002). While for the temperature function the air temperature can be used as an actual value, for the moisture function the actual vol. water content of the upper most numerical soil layer has to be used, since the moisture content of the soil-covering plant residues is assumed to be the same and is not simulated in an extra way. The carbon released during decomposition is partitioned by the factor $f_e(1-f_h)$ to microbial biomass, by the factor $f_e f_h$ to stabilized compounds of humus and by the factor $1-f_e$ to carbon dioxide. This is achieved using the parameter values known from the SOILN model: the efficiency factor f_e $[1]$ and the humus formation factor or humification factor f_h $[1]$. In contrast to the underlying model SOILN, the newly formed microbial biomass is fed exclusively to the surface pool of plant residues and it is assumed, that microbial biomass is also formed during the degradation of the above-ground humus pool.

The carbon balances of the surface pools therefore result from:

$$\frac{dC_{st}}{dt} = I_{st} - T_{st,ls} - U_{env}\,C_{st} \tag{641}$$

$$\begin{aligned}\frac{dC_{ls}}{dt} &= I_{ls} - T_{ls,lit} + T_{st,ls} + U_{env}\,C_{st} + \\ &\quad + f_e(1-f_h)\left(\frac{dC_{ls,dec}}{dt} + \frac{dC_{ms,dec}}{dt} + \frac{dC_{hs,dec}}{dt}\right) - \frac{dC_{ls,dec}}{dt}\end{aligned} \tag{642}$$

$$\frac{dC_{ms}}{dt} = I_{ms} - T_{ms,man} - \frac{dC_{ms,dec}}{dt} \tag{643}$$

$$\frac{dC_{hs}}{dt} = f_e\,f_h\left(\frac{dC_{ls,dec}}{dt} + \frac{dC_{ms,dec}}{dt}\right) - T_{hs,hum} - \frac{dC_{hs,dec}}{dt} \tag{644}$$

$$\frac{dC_{CO_2}}{dt} = (1-f_e)\left(\frac{dC_{ls,dec}}{dt} + \frac{dC_{ms,dec}}{dt}\right) + \frac{dC_{hs,dec}}{dt} \tag{645}$$

C_x	C-content $[kg\ ha^{-1}]$ of the surface pools $x = st, ls, ms, hs$ of organic matter
I_x	input function $[kg\ ha^{-1}\ d^{-1}]$ to the surface pool $x = st$ resp. soil pool $x = ls, ms$
$T_{x,y}$	transfer function $[kg\ ha^{-1}\ d^{-1}]$ from the surface pool $x = st, ls, ms, hs$ to the surface pool $x = st$ resp. to the soil pool $x = lit, man, hum$
$C_{x,dec}$	decomposed C-amount $[kg\ ha^{-1}]$ of the surface pool $x = st, ls, ms, hs$
C_{CO_2}	during decomposition of surface pools mineralised CO_2-carbon $[kg\ ha^{-1}]$
f_e	efficiency factor $[1]$
f_h	humification factor $[1]$
U_{env}	environmental impact rate $[d^{-1}]$ causing the transfer of standing to lying plant residues

3.5.4.3 N-Mineralisation at the Soil Surface The calculation of the N-turnover of the surface pools is carried out as in the model SOILN via the C/N-ratios of the pools and by the fixed C/N ratio r_0 of the microbial biomass formed during decomposition. However, the immobilisation is not reduced by N-limitation, but set to zero, if the available nitrogen is not sufficient to cover the N requirement of the microbes. In this case in the simulation no microbial growth takes place anymore and the total decomposed carbon is mineralised to CO_2, but by a reduced mineralisation rate. This reduction is simulated using a specific reduction factor f_{red} [1] (Berkenkamp et al., 2002):

$$f_{red} \;=\; \min\{\frac{r_0}{f_{C/N,x}}; f_e\} \tag{646}$$

The nitrogen-balances of the surface pools finally result from the following equations:

$$\frac{dN_{st}}{dt} \;=\; I_{st}^N - T_{st,ls}^N - U_{env}\, N_{st} \tag{647}$$

$$\begin{aligned} \frac{dN_{ls}}{dt} \;=\;& I_{ls}^N - T_{ls,lit}^N + T_{st,ls}^N + U_{env}\, N_{st} - \frac{1}{f_{C/N,ls}}\frac{dC_{ls,dec}}{dt} + \\ & \frac{f_e(1-f_h)}{r_0}\left(\frac{dC_{ls,dec}}{dt} + \frac{dC_{ms,dec}}{dt} + \frac{dC_{hs,dec}}{dt}\right) \end{aligned} \tag{648}$$

$$\frac{dN_{ms}}{dt} \;=\; I_{ms}^N - T_{ms,man}^N - \frac{1}{f_{C/N,ms}}\frac{dC_{ms,dec}}{dt} \tag{649}$$

$$\frac{dN_{hs}}{dt} \;=\; \frac{f_e\, f_h}{r_0}\left(\frac{dC_{ls,dec}}{dt} + \frac{dC_{ms,dec}}{dt}\right) - T_{hs,hum}^N - \frac{dC_{hs,dec}}{dt} \tag{650}$$

$$\frac{dN_{NH4}}{dt} \;=\; I_{NH4}^N \;+\; \Phi_{Min} \;-\; \Phi_{Imm,NH} \tag{651}$$

N_x	N-content $[kg\ ha^{-1}]$ of the specific surface pool $x = st, ls, ms, hs$ of organic matter
I_x^N	N-input function $[kg\ ha^{-1}\ d^{-1}]$ into surface resp. soil pools $x = st, ls, ms$
$T_{x,y}^N$	N-transfer function $[kg\ ha^{-1}\ d^{-1}]$ from the surface pool $x = st, ls, ms, hs$ in into the surface pool $x = st$ resp. into the soil pool $x = lit, man, hum$
$C_{x,dec}$	decomposed C-amount $[kg\ ha^{-1}]$ of the surface pool $x = st, ls, ms, hs$
N_{NH4}	during decomposition of the surface pool mineralised ammonium-N $[kg\ ha^{-1}]$
I_{NH4}^N	N-input $[kg\ ha^{-1}\ d^{-1}]$ by ammonium fertilizer to the soil surface
f_e, f_h	efficiency factor [1] and humification factor [1]
U_{env}	environmental impact rate $[d^{-1}]$ of transfer from standing to lying plant residues
$f_{C/N,x}$	C/N-ratio of surface pools $x = ls, ms, hs$ of organic matter
r_0	C/N-ratio of decomposing microbial biomass [1]
Φ_{Min}	ammonium-N source by mineralisation $[kg\ ha^{-1}\ d^{-1}]$ analogously to eq. (596)
$\Phi_{Imm,NH}$	ammonium-N sink by immobilisation $[kg\ ha^{-1}\ d^{-1}]$ analogously to eq. (597)

4 Water and Nitrogen Uptake by Roots

4.1 Root Water Uptake and Actual Transpiration

In many crop models the plant uptake of water and nitrogen from soil is mainly determined by the root distribution in the soil, the atmospheric water demand and the availability of soil water. Usually the actual daily water uptake is estimated by taking the minimum of three daily rates (given as water amounts per day): the water uptake capacity of the roots, the soil water availability and the atmospheric water demand.
The transpiration rate, at which plants extract water from soil is limited by the potential evapotranspiration rate, which describes the water demand by the atmosphere and thus is a measure of the available energy for water extraction by plants.

The actual water uptake by roots is influenced

- by the most often spatially and timely variable root distribution within the soil,
- by the rate at which the roots are supplied by water from the soil (i.e. by the water availability in the soil and thus indirectly by the matric potential h of the soil),
- by the flow resistance along the flow path from the soil-root interface through the plant to the atmosphere.

Therefore the actual transpiration rate and hence the water uptake by the plant is most often lower than the prescribed potential transpiration rate. In the literature various different soil physically and plant physiologically oriented models have been proposed (Molz, 1981). To these also belong the following empirical approaches:

4.1.1 Approach of the Model LEACHN

The sink term $S_w(t,z,h)$ $[mm\, mm^{-1}\, d^{-1}]$ of the Richards equation (103), which describes the root water uptake per unit soil volume, is determined according to Nimah and Hanks (1973) by the following equation:

$$S_w(t,z,h) \;=\; \beta(t,z)\; [K(h)\, \frac{\Delta H_{root/soil}}{\Delta x}]\; (\Delta z)^{-1} \tag{652}$$

$\frac{\Delta H_{root/soil}}{\Delta x}$	gradient of water potentials between roots and soil $[mm]$ (in the model the negative water potential $[kPa]$ is transformed into $[mm]$ pressure head)
$\beta(t,z)$	time and depth dependend root density distribution $[1]$
$K(h)$	unsaturated hydraulic conductivity $[mm\; d^{-1}]$ as a function of the soil matric potential h
Δx	half mean distance between roots
Δz	length of considered depth step

According to the Darcy-Buckingham law (97) the term in squared brackets describes the water flow between the root surface and a reference point x in the soil between the roots, at which the soil matric potential has been measured. It is assumed, that the distance Δx from x to the roots represents half of the mean distance between the roots.

To substitute the sink term into the discretised form of the Richards equation, also the sink term has to be discretised. For depth step i and the time interval from time step j-1 to j, this is achieved according to Nimah and Hanks (1973):

$$(S_w)_i^{j-1/2} = [H_{root} + i\Delta z\;(1 + R_c) - h_i^{j-1/2}][\beta_i^{j-1/2} K_i^{j-1/2}]/(\Delta z \Delta x) \qquad (653)$$

H_{root}	water potential in the root $[mm]$ at the soil surface (in the model the negative water potential $[kPa]$ is transformed into $[mm]$ pressure head)
$1 + R_c$	root resistance term $[1]$ to water flow in the root xylem
$h_i^{j-1/2} = (h_i^j + h_i^{j-1})/2$	matric potential $[mm]$ of the i-th soil layer during the time interval from $j-1$ to j calculated from the matric potentials h_{ij} and h_{ij-1} of the i-th soil layer at time steps j and $j-1$
$\beta_i^{j-1/2} = (\beta_i^j + \beta_i^{j-1})/2$	root length density $[mm\;mm^{-1}]$ of the i-th soil layer during the time interval between $j-1$ and j
$K_i^{j-1/2} = [K(h_i^j) + K(h_i^{j-1})]/2$	unsaturated hydraulic conductivity $[mm\;d^{-1}]$ of the i-th soil layer during the time interval between $j-1$ and j
Δz	thickness of the i-th soil layer $[mm]$
$\Delta x = 10\;mm$	distance $[mm]$ from the plant root to a point in the soil where the soil matric potentials h_i^j are measured

H_{root} is iteratively determined in a way, that the amount of water taken up by the root system during the time interval Δt, is equal to the water amount prescribed by the potential transpiration. To this end H_{root} takes values in the range between 0 and - 3000 kPa under the side condition that the soil cannot dry out below a matric potential of -1500 kPa caused by soil water extraction due to transpiration. Therefore, at dry soil conditions it is assumed that transpiration is restricted and ceases and the actual transpiration falls below the potential transpiration.

4.1.2 Approach of the Model CERES

In the models of the CERES model family the daily water uptake by the crop is calculated assuming a constant uptake rate for the whole day. The water uptake from the rooted soil layers is modeled by prescribing a maximal possible potential root water uptake. The important factors, that determine the potential root water uptake, are the hydraulic conductivities of the soil layers and the root resistance, which characterizes the water permeability of the roots. By the root resistance an upper limit to water uptake exists, which is considered by a maximal daily root water uptake per unit root length and unit soil depth given by $A_W^{max} = 3.0 \;\; mm^3 \; mm^{-1} \; d^{-1}$. The daily potential root water availability or supply rate per unit root length and unit soil depth $A_{W,i}^{pot}$ $[mm^3 \; mm^{-1} \; d^{-1}]$ is calculated by

$$A_{W,i}^{pot} = 2.67 \; 10^{-3} \; - \; 3.0 \; \exp[62.0 \; (\theta_i - \theta_{pwp,i})]/[6.68 \; - \; \ln(l_i)] \tag{654}$$

$A_{W,i}^{pot}$	daily potential root water availability rate $[mm^3 \; mm^{-1} \; d^{-1}]$ per millimeter root length from the i-th soil layer
θ_i	vol. water content $[mm^3 \; mm^{-3}]$ of the i-th soil layer
$\theta_{pwp,i}$	vol. water content at the permanent wilting point $[mm^3 \; mm^{-3}]$ of the i-th soil layer
l_i	root length density $[mm \; mm^{-3}]$ of the i-th soil layer

The equation for water availability was derived from a model describing radial water flow towards a single root assuming all soils have similar hydraulic conductivities near the permanent wilting point. It is also assumed that the calculation is of sufficient accuracy if only a constant water potential gradient between the root and the soil is considered (Jones and Kiniry, 1986; Ritchie et al., 1987), see also Wang and Smith (2004) for details. The daily potential root uptake rate A_i^{pot} $[mm \; d^{-1}]$ from the i-th soil layer then results from

$$A_i^{pot} \; = \; \min(A_W^{max}; A_{W,i}^{pot}) \; d_i \; l_i \tag{655}$$

A_i^{pot}	daily potential root water uptake rate $[mm \; d^{-1}]$ from the i-th soil layer
A_W^{max}	maximal daily root water uptake rate $[mm^3 \; mm^{-1} \; d^{-1}]$ per millimeter root length
$A_{W,i}^{pot}$	daily potential root water uptake rate $[mm^3 \; mm^{-1} \; d^{-1}]$ per millimeter root length of the i-th soil layer
d_i	thickness of the i-th soil layer $[mm]$
l_i	root length density $[mm \; mm^{-3}]$ of the i-th soil layer

By summation of the layer related rates the total daily potential root water uptake rate A_{pot}^{day} $[mm\ d^{-1}]$ from the rooted soil profile is calculated:

$$A_{pot}^{day} \ = \ \sum_i A_i^{pot} \tag{656}$$

A_{pot}^{day}	daily potential root water uptake rate $[mm\ d^{-1}]$ from the rooted soil layers
A_i^{pot}	daily potential root water uptake rate $[mm\ d^{-1}]$ from the i-th soil layer

The daily actual root water uptake rate A_i^{act} $[mm\ d^{-1}]$ from the i-th soil layer is then given by reducing the uptake to the water demand of the crop, which is prescribed by the daily potential transpiration rate TR_{pot}^{day} $[mm\ d^{-1}]$ and represents the corresponding atmospheric water demand:

$$A_i^{act} \ = \ A_i^{pot} \ \min(1.0 \ ; \ TR_{pot}^{day}/A_{pot}^{day}) \tag{657}$$

A_i^{act}	daily actual root water uptake rate $[mm\ d^{-1}]$ from the i-th soil layer
A_i^{pot}	daily potential root water uptake rate $[mm\ d^{-1}]$ from the i-th soil layer
TR_{pot}^{day}	daily potential transpiration rate $[mm\ d^{-1}]$
A_{pot}^{day}	daily potential root water uptake rate $[mm\ d^{-1}]$ from the rooted soil layers

For the crop growth model additionally two soil water deficit factors are defined, describing water stress for growth $f_{\theta,1}$ $[-]$ and photosynthesis $f_{\theta,2}$ $[-]$:

$$f_{\theta,1} = \min(1.0 \ ; \ A_{pot}^{day}/TR_{pot}^{day}), \qquad f_{\theta,2} = \frac{2}{3}\min(1.5 \ ; \ A_{pot}^{day}/TR_{pot}^{day}) \tag{658}$$

Finally the daily actual transpiration rate is calculated according to:

$$TR_{day}^{akt} = \begin{cases} TR_{pot}^{day} & \text{for } f_{\theta,1} = 1 \\ A_{pot}^{day} & \text{for } f_{\theta,1} < 1 \end{cases} \tag{659}$$

TR_{pot}^{day}	daily potential transpiration rate $[mm\ d^{-1}]$
A_{pot}^{day}	daily potential root water uptake rate $[mm\ d^{-1}]$ from the rooted soil layers

4.1.3 Approach of the Model SWATRE

In the model SWATRE of Belmans et al. (1983) the sink term $S_w(t,z,h)$ $[mm\, mm^{-1}\, d^{-1}]$ of the Richards equation (103), which describes the root water uptake per unit time and unit soil volume, is calculated according to the approach of Feddes et al. (1978), see also Vogel et al. (1996), by

$$S_w(t,z,h) = \alpha(t,z,h)\; S_{max}(t,z) \tag{660}$$

where $\alpha(t,z,h)$ $[-]$ is a water stress function depending on time t, soil depth z and matric potential h, and where $S_{max}(t,z)$ $[d^{-1}]$ denotes the maximal water uptake rate from the rooted soil profile.

Since usually the distribution of the roots within the soil profile is non-uniform, also the maximal water uptake rate is non-uniformly distributed over the rooted soil profile and hence may be described by:

$$S_{max}(t,z) = \beta(t,z)\; TR_{pot}(t) \tag{661}$$

$S_{max}(t,z)$	time and depth dependent maximal root uptake rate $[d^{-1}]$ from the rooted soil profile
$\beta(t,z)$	time and depth dependent potential water uptake distribution $[mm^{-1}]$
$TR_{pot}(t)$	potential transpiration rate $[mm\; d^{-1}]$ at time t

The function $\beta(t,z)$ $[mm^{-1}]$ gives the vertical distribution of the potential water uptake in the rooted soil. It is often obtained by normalisation of the root density distribution, which is assumed to be directly proportional to the distribution of the potential root water uptake $\tilde{\beta}(t,z)$:

$$\beta(t,z) = \frac{\tilde{\beta}(t,z)}{\displaystyle\int_0^{\ell_r} \tilde{\beta}(t,z)dz} \tag{662}$$

$\beta(t,z)$	time and depth dependent potential water uptake distribution $[mm^{-1}]$
$\tilde{\beta}(t,z)$	time and depth dependent potential root water uptake distribution $[1]$ or root density distribution $[1]$
ℓ_r	depth of the root zone $[mm]$ at time t

Applying these definitions the potential transpiration rate $TR_{pot}(t)$ at time t can be expressed via the maximal water uptake rate $S_{max}(t,z)$:

$$\int_0^{\ell_r} S_{max}(t,z)\; dz = \int_0^{\ell_r} \beta(t,z)\; TR_{pot}(t)\; dz = TR_{pot}(t) \tag{663}$$

Then by inserting equation (660) and equation (661) into equation (663) also the actual transpiration rate $TR_{act}(t)$ $[mm\ d^{-1}]$ at time t can be calculated:

$$\begin{aligned} TR_{act}(t) = \int_0^{\ell_r} S_w(t,z,h)\ dz &= \int_0^{\ell_r} S_{max}(t,z)\ \alpha(t,z,h)\ dz \\ &= TR_{pot}(t) \int_0^{\ell_r} \alpha(t,z,h)\ \beta(t,z)\ dz \end{aligned} \tag{664}$$

To this end, the water stress function $\alpha(t,h)$ according to Feddes et al. (1978) is defined by:

$$\alpha(t,h) = \begin{cases} 0 & \text{for } h < h_3 \\ \dfrac{h - h_3}{h_2(t) - h_3} & \text{for } h_3 \leq h < h_2(t) \\ 1 & \text{for } h_2(t) \leq h < h_1 \\ \dfrac{h - h_0}{h_1 - h_0} & \text{for } h_1 \leq h < h_0 \\ 0 & \text{for } h_0 \leq h \end{cases} \tag{665}$$

$\alpha(t,h)$	time and depth dependent water stress function $[1]$
h_0	matric potential $[mm]$ above which die water uptake ceases (also called point of anaerobiosis)
h_1	matric potential $[mm]$ below which water uptake starts to be optimal
h_2	matric potential $[mm]$ below which water uptake stops to be optimal
h_3	matric potential $[mm]$ below which no water uptake occurs (usually corresponds to the wilting point)

Here h_0 to h_3 denote prescribed values (input parameters) representing soil matric potentials. It is assumed that water uptake ceases if the soil is extremely wet ($h \geq h_0$) because root respiration is confined due to restricted oxygen supply from the atmosphere. At soil matric potential between h_1 and h_2 the root water uptake is assumed to be optimal. At the dry end, below the wilting point given by h_3, no water uptake occurs. Between the regions of optimal and no water uptake a linear interpolation is used.

The value h_2 representing the matric potential at drier soil conditions, where the water uptake is not anymore optimal, depends on the potential transpiration at time t. h_2 is higher at high water demand of the plants, it is lower at low water demand. This is calculated by the following relation (Wesseling and Brandyk, 1985; Vogel et al., 1996):

$$h_2 = \begin{cases} h_{2L} & \text{for } TR_{pot}(t) < TR_{potL} \\ h_{2L} + \dfrac{TR_{potH} - TR_{pot}(t)}{TR_{potH} - TR_{potL}}\,(h_{2H} - h_{2L}) & \text{for } TR_{potL} \leq TR_{pot}(t) \leq TR_{potH} \\ h_{2H} & \text{for } TR_{potH} < TR_{pot}(t) \end{cases} \tag{666}$$

h_2	matric potential $[mm]$ below which the water uptake stops to be optimal
h_{2L}	matric potential $[mm]$ for h_2 at low transpiration demand
h_{2H}	matric potential $[mm]$ for h_2 at high transpiration demand
$TR_{pot}(t)$	potential transpiration $[mm\ d^{-1}]$ at time t
TR_{potL}	lower limit of potential transpiration $[mm\ d^{-1}]$ for the determination of h_2
TR_{potH}	upper limit of potential transpiration $[mm\ d^{-1}]$ for the determination of h_2

4.1.4 Approach of the Model HYDRUS

An alternative function to the water stress function of Feddes et al. (1978) was proposed by van Genuchten (Vogel et al., 1996):

$$\alpha(t,h) = \frac{1}{1\ +\ (h/h_{50})^P} \tag{667}$$

$\alpha(t,h)$	time and depth dependent water stress function [1]
h	matric potential $[mm]$ of the soil
h_{50}	matric potential $[mm]$ at which the water uptake rate is reduced by 50 %
P	empirical constant, that influences the slope of the curve [1] (e.g. P=3).

This water stress function can be applied instead of the function of Feddes. But then, if the soil is almost at water saturation, the reduced water uptake at oxygen shortage is not considered.

4.2 Root N-Uptake

4.2.1 Approach of the Model LEACHN

In the model LEACHN the simulation of root N-uptake by different plant species is performed following Watts and Hanks (1978). To this end, for each plant species the potential total N-uptake $N_{upt}^{pot,tot}$ $[kg\ N\ ha^{-1}]$ during the considered vegetation period has to be given as input. From this input the daily potential N-uptake rate $(\frac{dN_{upt}}{dt})_{pot}^{day},\ \ [kg\ N\ ha^{-1}d^{-1}]$ of the crop canopy is determined.

First the potential N-uptake f_{tnu} [1] as fraction of the potential total N-uptake is estimated by an empirical regression equation using the fraction f_{gs} [1] of the time interval passed since the begin of the vegetation period in relation to the time interval of the whole vegetation period, i.e. from its begin t_{beg} $[d]$ until its end t_{end} $[d]$:

$$f_{gs} = (t + 1 - t_{beg})/(t_{end} - t_{beg}) \tag{668}$$

$$f_{tnu} = \begin{cases} 8,9\ f_{gs}^{3,87} & \text{for } 0 \leq f_{gs} < 0,3 \\ -0,66\ f_{gs} + 3,49\ f_{gs}^2 - 0,93\ f_{gs}^3 - 0,9\ f_{gs}^4 & \text{for } 0,3 \leq f_{gs} \leq 1,0 \end{cases} \tag{669}$$

The daily potential N-uptake rate $(\frac{dN_{upt}}{dt})_{pot}^{day},\ \ [kg\ N\ ha^{-1}d^{-1}]$ then results from the difference between the potential N-uptake at actual time and the already performed cumulative N-uptake $N_{up}^{act,cum}$ $[kg\ N\ ha^{-1}]$ by the crop, where the difference is related to the whole day (Δt = 1 d), i.e. is considered as a rate per day. At the end of the vegetation period ($f_{gs} > 0,7$), when the plants cannot anymore compensate a possible N-deficit, the potential N-uptake rate is reduced:

$$\left(\frac{dN_{upt}}{dt}\right)_{pot}^{day} = \begin{cases} (N_{upt}^{pot,tot} f_{tnu} - N_{upt}^{act,cum})/\Delta t, & f_{gs} \leq 0.7 \\ [(N_{upt}^{pot,tot} f_{tnu} - N_{upt}^{act,cum})/\Delta t]\ [\frac{1-(f_{gs}-0.7)}{0.3}], & f_{gs} > 0.7 \end{cases} \tag{670}$$

The actual N-uptake rate $(\frac{dN_{upt}}{dt})_{act}^{\Delta t},\ \ [kg\ N\ ha^{-1}d^{-1}]$ during the time interval Δt is finally determined as sum of the nitrate-N and ammonium-N uptake rates from the root zone (of maximal rooting depth z_{max} $[dm]$) which depend on the actual soil solution concentrations c_I $[mg\ dm^{-3}]$ of nitrate-N ($I = NO$) and ammonium-N ($I = NH$):

$$\left(\frac{dN_{upt}}{dt}\right)_{act}^{\Delta t} = \sum_{I=NH,NO} \int_0^{z_{max}} \min\{\ \frac{1}{2}\ \theta\ c_I/\Delta t,\ \left(\frac{dN_{upt}}{dt}\right)_{pot}^{day} f_{TR}\ f_{NU,I}\ \}\ dz \tag{671}$$

$$f_{TR} = TR_p^{\Delta t} /\ TR_{pot}^{day}\ , \qquad f_{NU,I} = S_w\ c_I\ /\ \int_0^{z_{max}} [S_w\ (c_{NO} + c_{NH})]\ dz \tag{672}$$

θ vol. water content [1] , S_w water uptake rate $[d^{-1}]$ by transpiration , $TR_p^{\Delta t}$ potential transpiration rate $[mm\ d^{-1}]$ during the time interval Δt , TR_{pot}^{day} daily potential transpiration rate $[mm\ d^{-1}]$

4.2.2 Approach of the Model CERES-N

In the CERES models the nitrogen which is potentially accessible by roots is described in analogy to the available water by use of availability factors per unit root length of the i-th rooted soil layer, i.e. by $f^{avl}_{NO_3,i}$ $[-]$ for nitrate-N and $f^{avl}_{NH_4,i}$ $[-]$ for ammonium-N. These N availability factors are estimated by empirical relationships using crop specific nitrate-N and ammonium-N accessibility factors (input parameters) γ_{c,NO_3} $[-]$ and γ_{c,NH_4} $[-]$:

$$f^{avl}_{NO_3,i} = 1 - \exp(\gamma_{c,NO_3}\, C_{NO_3,i}), \tag{673}$$

$$f^{avl}_{NH_4,i} = 1 - \exp(\gamma_{c,NH_4}\, C_{NH_4,i}) \tag{674}$$

where $C_{NO_3,i}$ $[kg\ N\ ha^{-1}]$ and $C_{NH_4,i}$ $[kg\ N\ ha^{-1}]$ denote the nitrate-N and ammonium-N amounts of the i-th soil layer.

Furthermore, it is assumed, that there exist upper limits to root N-uptake, that are given by crop specific maximal uptake rates per unit root length: $A^{max}_{NO_3}$ $[\mu g\ N\ cm^{-1}\ d^{-1}]$ for soil nitrate-N uptake and $A^{max}_{NH_4}$ $[\mu g\ N\ cm^{-1}\ d^{-1}]$ for ammonium-N uptake (input parameters).

The daily potential root uptake rates $A^{pot}_{NO_3,i}$ of nitrate-N $[kg\ N\ ha^{-1}\ d^{-1}]$ and $A^{pot}_{NH_4,i}$ of ammonium-N $[kg\ N\ ha^{-1}\ d^{-1}]$ from the i-th soil layer are then defined by:

$$A^{pot}_{NO_3,i} = A^{max}_{NO_3}\, f^{avl}_{NO_3,i}\, f_{\theta,i}\, d_i\, l_i \tag{675}$$

$$A^{pot}_{NH_4,i} = A^{max}_{NH_4}\, f^{avl}_{NH_4,i}\, f_{\theta,i}\, d_i\, l_i \tag{676}$$

$A^{pot}_{NO_3,i}$	daily potential root uptake rate of nitrate-N $[mm^3\ mm^{-1}\ d^{-1}]$ from the i-th soil layer
$A^{pot}_{NH_4,i}$	daily potential root uptake rate of ammonium-N $[mm^3\ mm^{-1}\ d^{-1}]$ from the i-th soil layer
$A^{max}_{NO_3}$	maximal root uptake rate of nitrate-N $[\mu g\ N\ cm^{-1}\ d^{-1}]$
$A^{max}_{NH_4}$	maximal root uptake rate of ammonium-N $[\mu g\ N\ cm^{-1}\ d^{-1}]$
$f^{avl}_{NO_3,i}$	availability factor of nitrate-N $[-]$ of the i-th soil layer
$f^{avl}_{NH_4,i}$	availability factor of ammonium-N $[-]$ of the i-th soil layer
l_i	root length density $[mm\ mm^{-3}]$ of the i-th soil layer
d_i	thickness $[mm]$ of the i-th soil layer

where the soil moisture deficit factor $f_{\theta,i}$ $[-]$ of the i-th soil layer is given by

$$f_{\theta,i} = (\theta_i - \theta_{pwp,i})/(\theta_{fc,i} - \theta_{pwp,i}) \tag{677}$$

θ_i	vol. water content $[mm^3\ mm^{-3}]$ of the i-th soil layer
$\theta_{pwp,i}$	vol. water content at the permanent wilting point $[mm^3\ mm^{-3}]$ of the i-th soil layer
$\theta_{fc,i}$	vol. water content at field capacity $[mm^3\ mm^{-3}]$ of the i-th soil layer

The total daily potential nitrate-N uptake rate A^{day}_{pot,NO_3} $[kg\ N\ ha^{-1}\ d^{-1}]$ and the total daily potential ammonium-N uptake rate A^{day}_{pot,NH_4} $[kg\ N\ ha^{-1}\ d^{-1}]$ result as the sum of the corresponding uptake rates of each rooted soil layer:

$$A^{pot}_{NO_3} \quad = \quad \sum_i A^{pot}_{NO_3,i}, \qquad A^{pot}_{NH_4} \; = \; \sum_i A^{pot}_{NH_4,i} \tag{678}$$

$A^{pot}_{NO_3}$	daily potential nitrate-N uptake rate $[kg\ N\ ha^{-1}\ d^{-1}]$ from the rooted soil layers
$A^{pot}_{NO_3,i}$	daily potential nitrate-N uptake rate $[kg\ N\ ha^{-1}\ d^{-1}]$ from the i-th soil layer
$A^{pot}_{NH_4}$	daily potential ammonium-N uptake rate $[kg\ N\ ha^{-1}\ d^{-1}]$ from the rooted soil layers
$A^{pot}_{NH_4,i}$	daily potential ammonium-N uptake rate $[kg\ N\ ha^{-1}\ d^{-1}]$ from the i-th soil layer

and from these the total daily potential mineral N uptake rate $A^{day}_{pot,N_{min}}$ $[kg\ N\ ha^{-1}\ d^{-1}]$ is obtained using:

$$A^{day}_{pot,N_{min}} = A^{day}_{pot,NO_3} + A^{day}_{pot,NH_4} \tag{679}$$

Thus, an actual nitrogen uptake factor $f_{act,N}$ $[-]$ can be defined that relates the total daily N-demand $D^{day}_{c,N}$ of the crop $[kg\ N\ ha^{-1}\ d^{-1}]$ to the total daily potential N-uptake:

$$f_{act,N} = \min\{1.0,\ D^{day}_{c,N}/A^{day}_{pot,N_{min}}\} \tag{680}$$

The factor is used to reduce the potential N-uptake if the N-demand is lower than the potential uptake for computing the actual daily nitrate-N uptake $A^{act}_{NO_3,i}$ $[kgN\ ha^{-1}\ d^{-1}]$ and ammonium-N uptake $A^{act}_{NH_4,i}$ $[kgN\ ha^{-1}\ d^{-1}]$ from the i-th soil layer:

$$A^{act}_{NO_3,i} \quad = \quad \min\{A^{pot}_{NO_3,i}\ f_{act,N},\ C_{NO_3,i} - C_{NO_3,min}\} \tag{681}$$

$$A^{act}_{NH_4,i} \quad = \quad \min\{A^{pot}_{NH_4,i}\ f_{act,N},\ C_{NH_4,i} - C_{NH_4,min}\} \tag{682}$$

$A^{pot}_{NO_3,i}$	daily potential root uptake rate of nitrate-N $[mm^3\ mm^{-1}\ d^{-1}]$ from the i-th soil layer
$A^{pot}_{NH_4,i}$	daily potential root uptake rate of ammonium-N $[mm^3\ mm^{-1}\ d^{-1}]$ from the i-th soil layer
$f_{act,N}$	actual nitrogen uptake factor $[-]$
$C_{NO_3,i}$	nitrate-N amount $[kg\ N\ ha^{-1}]$ of the i-th soil layer
$C_{NH_4,i}$	ammonium-N amount $[kg\ N\ ha^{-1}]$ of the i-th soil layer
$C_{NO_3,min}$	minimal nitrate-N amount $[kg\ N\ ha^{-1}]$ of the i-th soil layer which cannot be extracted by the crop
$C_{NH_4,min}$	minimal ammonium-N amount $[kg\ N\ ha^{-1}]$ of the i-th soil layer which cannot be extracted by the crop

The pattern of nitrogen extraction among the rooted soil layers therefore is from each soil layer according to the ratio of available amounts within the root zone. Hence, uptake is from the layers with higher nitrogen contents.

4.2.3 Approach of the Model EXPERT-N

Similar to the approach of the model LEACHN following Watts and Hanks (1978) also in the model EXPERT-N N-uptake of different crops can be simulated. In a more general way it is assumed that for each plant species not only the potential total N-uptake $N_{upt}^{pot,tot}$ $[kg\ N\ ha^{-1}]$ of the entire vegetation period is known, but also the cumulative potential N-uptake $N_{upt,i}^{pot,cum}$ $[kg\ N\ ha^{-1}]$ at additional times t_i $[d]$, $2 \leq i \leq n$ during the vegetation period. By interpolation between the different potential cumulative N-uptake values it is then possible to estimate an actual N-uptake rate $(\frac{dN_{upt}}{dt})_{pot}^{\Delta t}$, $[kg\ N\ ha^{-1}d^{-1}]$ of the crop during the time interval Δt $[d]$.

At first for the actual time t $[d]$, which lies between two dates t_i, where cumulative N-uptake is known ($t_{i-1} \leq t < t_i$), the fraction of the potential N-uptake f_{tnu} [1] of the potential cumulative N-uptake at t_i is determined by the time fraction f_{gs} [1] of the already passed time between t_{i-1} and t_i:

$$f_{gs} = (t + 1 - t_{i-1})/(t_i - t_{i-1}) \tag{683}$$

$$f_{tnu} = \begin{cases} 5,556\ f_{gs}^2 & \text{for } 0 \leq f_{gs} < 0,3 \\ -\ f_{gs}^2 + 2\ f_{gs} & \text{for } 0,3 \leq f_{gs} \leq 1,0 \end{cases} \tag{684}$$

The potential cumulative N-uptake $N_{up}^{pot,cum}$ $[kg\ N\ ha^{-1}]$ at time t then results from

$$N_{up}^{pot,cum} = f_{tnu}\ (N_{up,i+1}^{pot,cum} - N_{up,i}^{pot,cum})\ +\ N_{up,i}^{pot,cum} \tag{685}$$

Finally the actual N-uptake rate $(\frac{dN_{upt}}{dt})_{act}^{\Delta t}$, $[kg\ N\ ha^{-1}d^{-1}]$ during the time step $\Delta t \leq 1d$ is calculated as the sum of the corresponding nitrate-N and ammonium-N uptake rates from the root zone (of rooting depth z_{max} $[dm]$). These rates are determined depending on the soil N-amounts N_I $[kg\ N\ ha^{-1}]$ of nitrate $I = NO$ and ammonium $I = NH$, on the root length density γ_{root} $[mm\ dm^{-3}]$ and on the crop N-demand N_{up}^{dem} $[kg\ N\ ha^{-1}]$ given as the difference between the potential cumulative N-uptake $N_{up}^{pot,cum}$ $[kg\ N\ ha^{-1}]$ and the actual cumulative N-uptake $N_{up}^{act,cum}$ $[kg\ N\ ha^{-1}]$, which has already taken place. With it, it is assumed, that the soil can only be depleted to a minimal N-amount N_{min} $[kg\ N\ ha^{-1}]$:

$$\left(\frac{dN_{upt}}{dt}\right)_{act}^{\Delta t} = \sum_{I=NH,NO} \int_0^{z_{max}} \min\{N_I - N_{min},\ N_I\ f_{NU}\ N_{up}^{dem}\ \gamma_{root}\}\ dz\ /\Delta t \tag{686}$$

$$N_{up}^{dem} = N_{up}^{pot,cum} - N_{up}^{act,cum}\ , \qquad f_{NU}^{-1} = \int_0^{z_{max}} (N_{NO} + N_{NH})\ \gamma_{root}\ dz \tag{687}$$

4.2.4 Approach of the Models WHNSIM and WAVE

In the models WHNSIM (Huwe, 1992) and WAVE (Vanclooster et al., 1994) the daily actual N-uptake rate $(\frac{dN_{upt}}{dt})^{day}_{act}$ of a crop canopy $[kg\ N\ ha^{-1}\ d^{-1}]$ is modeled based on the approach of McIsaac et al. (1985).

Here, the daily actual N-uptake rate $(\frac{dN_{upt}}{dt})^{day}_{act}$ results

- from the N-uptake by convection $(\frac{dN_{upt}}{dt})^{day}_{conv}$, $[kg\ N\ ha^{-1}\ d^{-1}]$, i.e. the mineral N-uptake from the soil solution by water uptake due to the transpiration flux,
- and from the N-uptake by diffusion $(\frac{dN_{upt}}{dt})^{day}_{diff}$, $[kg\ N\ ha^{-1}\ d^{-1}]$, due to diffusion of mineral N into the plant roots:

$$\left(\frac{dN_{upt}}{dt}\right)^{day}_{act} = \left(\frac{dN_{upt}}{dt}\right)^{day}_{conv} + \left(\frac{dN_{upt}}{dt}\right)^{day}_{diff} \tag{688}$$

The actual N-uptake is limited by the maximal possible N-uptake during the course of the day, i.e. by the daily potential N-uptake rate $(\frac{dN_{upt}}{dt})^{day}_{pot}$, $[kg\ N\ ha^{-1}\ d^{-1}]$. If the growth of the canopy is directly simulated by a crop growth model, the potential N-uptake is derived from the N-demand of the plant organs:

$$\left(\frac{dN_{upt}}{dt}\right)^{day}_{pot} = \left(\frac{dN_{upt}}{dt}\right)^{day}_{dem,lvs} + \left(\frac{dN_{upt}}{dt}\right)^{day}_{dem,sts} + \left(\frac{dN_{upt}}{dt}\right)^{day}_{dem,rts} \tag{689}$$

where $(dN_{upt}/dt)^{day}_{dem,lvs}$, $(dN_{upt}/dt)^{day}_{dem,sts}$ and $(dN_{upt}/dt)^{day}_{dem,rts}$ respectively denote the daily N-demand of the leaves, stems and roots in $[kg\ N\ ha^{-1}\ d^{-1}]$.

If not directly simulated by the growth model, the daily N-demand of the plant organs can also be calculated by the following approach:

$$\left(\frac{dN_{upt}}{dt}\right)^{day}_{pot,lvs} = B_{lvs}\ f_{N,lvs} - N_{lvs} \tag{690}$$

$$\left(\frac{dN_{upt}}{dt}\right)^{day}_{pot,sts} = B_{sts}\ f_{N,sts} - N_{sts} \tag{691}$$

$$\left(\frac{dN_{upt}}{dt}\right)^{day}_{pot,rts} = B_{rts}\ f_{N,rts} - N_{rts} \tag{692}$$

$B_{lvs}, B_{sts}, B_{rts}$	biomass dry weight $[kg\ ha^{-1}]$ of leaves, stems, respectively roots
$f_{N,lvs}, f_{N,sts}, f_{N,rts}$	potential N-fraction [1] of the leaves, stems, respectively roots, where $f_{N,lvs}$ is given as an input parameter depending on the development stage and where additionally $f_{N,sts} = f_{N,rts} = \frac{1}{2}\ f_{N,lvs}$ is assumed.
$N_{lvs}, N_{sts}, N_{rts}$	accumulated N $[kg\ ha^{-1}]$ in leaves, stems, respectively roots.

The actual daily convective N-uptake $(\frac{dN_{upt}}{dt})^{day}_{conv}$, $[kg\ N\ ha^{-1}\ d^{-1}]$ is calculated from the nitrate-N concentration c_{NO_3} $[mg\ dm^{-3}]$ and the ammonium-N concentration c_{NH_4} $[mg\ dm^{-3}]$ in the soil solution taken up by the roots with the transpiration flux represented by the sink term S_w $[mm\ d^{-1}]$, where z_{max} denotes the maximal rooting depth:

$$\Big(\frac{dN_{upt}}{dt}\Big)^{day}_{conv} = \int_0^{z_{max}} \Big[\int_0^1 S_w\ (c_{NO} + c_{NH})\ dt\Big]\ dz \tag{693}$$

where the inner integral represents the cumulative uptake of water and mineral N during the whole day and the outer integral is over the spatial region of the entire root zone.

If the calculated convective N-uptake rate is higher than the potential N-uptake rate, then no diffusive N-uptake is determined and the daily actual N-uptake is reduced to the potential N-uptake. Otherwise, if the N-demand of the crop is higher than the convective N-uptake, at first the daily potential diffusive N-uptake rate $(\frac{dN_{upt}}{dt})^{day}_{pot}$, [kg N ha^{-1} d^{-1}] is computed:

$$\Big(\frac{dN_{upt}}{dt}\Big)^{day}_{pot,diff} = \Big(\frac{dN_{upt}}{dt}\Big)^{day}_{pot} - \Big(\frac{dN_{upt}}{dt}\Big)^{day}_{conv} \tag{694}$$

In the next step, the daily maximal N-uptake rate by diffusion $(\frac{dN_{upt}}{dt})^{day}_{max,diff}$, $[kg\ N\ ha^{-1}\ d^{-1}]$ is determined by deriving the radial diffusive flux into a cylindrical root:

$$\Big(\frac{dN_{upt}}{dt}\Big)^{day}_{max,diff} = \int_0^{z_{max}} 2\pi r_{root}\gamma_{root}\ D(\theta)\ \frac{\theta\ (c_{NO} + c_{NH}) - c_{rs}}{10^6\ l_d}\ dz \tag{695}$$

Here the N-uptake is calculated considering (i) the root surface $2\pi r_{root}\gamma_{root}$ $[mm^2\ dm^{-3}]$ per unit soil volume determined by the average root radius r_{root} $[mm]$ and the root length density γ_{root} $[mm\ dm^{-3}]$, (ii) the diffusive flux given by the diffusion coefficient $D(\theta)$ $[mm^2\ d^{-1}]$ for diffusion within the soil, and by the concentration gradient between the N$_{min}$-concentration $c_{NO} + c_{NH}$ $[mg\ dm^{-3}]$ in the soil solution surrounding the root and the N$_{min}$-concentration at the root surface c_{rs} $[mg\ dm^{-3}]$, which is zero ($c_{rs} = 0$) in case of maximal diffusive N-uptake. Thereby l_d $[mm]$ denotes the characteristic diffusion length of 0.1 mm between root surface and soil solution at a point of average soil solution concentration. The factor 10^{-6} is to convert $[mm^3]$ into $[dm^3]$ and θ [1] denotes the volumetric soil water content.

Finally the daily actual diffusive N-uptake results by:

$$\Big(\frac{dN_{upt}}{dt}\Big)^{day}_{diff} = \min\Big\{\Big(\frac{dN_{upt}}{dt}\Big)^{day}_{pot,diff}\ ;\ \Big(\frac{dN_{upt}}{dt}\Big)^{day}_{max,diff}\Big\} \tag{696}$$

Collectively, the daily actual N-uptake rate $(\frac{dN_{upt}}{dt})^{day}_{act}$ then results from equation (688).

The daily actual N-uptake rate $(\frac{dN_{upt}}{dt})^{day}_{act,x}$, $[kg\ N\ ha^{-1}\ d^{-1}]$ into the particular plant organs $x = lvs, sts, rts$ (leaves, stems, roots) results from the total N-uptake rate and the respective fraction of the plant organs N-demand at the total N-demand, see also the above equations (690)- (693):

$$\left(\frac{dN_{upt}}{dt}\right)^{day}_{act,lvs} = \left(\frac{dN_{upt}}{dt}\right)^{day}_{pot,lvs} \frac{\left(\frac{dN_{upt}}{dt}\right)^{day}_{act}}{\left(\frac{dN_{upt}}{dt}\right)^{day}_{pot}} - \left(\frac{dN_{upt}}{dt}\right)^{day}_{sto} \left(\frac{B_{lvs}}{B_{lvs} + B_{sts}}\right) \tag{697}$$

$$\left(\frac{dN_{upt}}{dt}\right)^{day}_{act,sts} = \left(\frac{dN_{upt}}{dt}\right)^{day}_{pot,sts} \frac{\left(\frac{dN_{upt}}{dt}\right)^{day}_{act}}{\left(\frac{dN_{upt}}{dt}\right)^{day}_{pot}} - \left(\frac{dN_{upt}}{dt}\right)^{day}_{sto} \left(\frac{B_{sts}}{B_{lvs} + B_{sts}}\right) \tag{698}$$

$$\left(\frac{dN_{upt}}{dt}\right)^{day}_{act,rts} = \left(\frac{dN_{upt}}{dt}\right)^{day}_{pot,rts} \frac{\left(\frac{dN_{upt}}{dt}\right)^{day}_{act}}{\left(\frac{dN_{upt}}{dt}\right)^{day}_{pot}} \tag{699}$$

$$\left(\frac{dN_{upt}}{dt}\right)^{day}_{sto} = (B_{sto}\, f_{N,sto} - N_{sto})\, f_{red} \tag{700}$$

$$\text{with reduction factor} \quad f_{red} = 1 - \sqrt{1 - f^2_{N,red}}\,, \quad f_{N,red} = \frac{g_{N,lvs} - h_{N,lvs}}{l_{N,lvs} - h_{N,lvs}} \tag{701}$$

B_{sto}	biomass dry weight $[kg\ ha^{-1}]$ of storage organs
$f_{N,sto}$	potential N-fraction [1] of storage organs, where $f_{N,sto}$ is an input parameter depending on development stage and plant species.
N_{sto}	accumulated N $[kg\ ha^{-1}]$ in storage organs
$g_{N,lvs}$	actual N-fraction [1] of the leaves
$h_{N,lvs}$	threshold value of the N-fraction of leaves [1] above which optimal growth occurs and for which $h_{N,lvs} = \frac{1}{2} f_{N,lvs}$ is assumed.
$l_{N,lvs}$	threshold value of the N-fraction of leaves [1] below which no more growth occurs and for which the value $l_{N,lvs} = 0.005$ is assumed.

5 Growth Models for Agricultural Crops

5.1 Introduction

5.2 CERES Growth Models

5.3 SPASS Growth Models

5.4 SUCROS Growth Models

5.5 GECROS Growth Models

6 Growth Models for Forestal Crops

6.1 TREEDYN Growth Models

6.2 FAGUS Growth Model

7 Growth Models for Agro-Forest Systems

8 Growth Models for Individual Plants

8.1 PLATHO Growth Model

8.2 PLAWAT Flow and Transport Model

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