CANDY 22 MANUAL III

Description of Background



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Software available for download at **www.frug.info/candy_main.php**

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Preliminary notes

This document is intended to help potential users to understand how the model is working and to provide first assistance working with the code. The candy app is written in PASCAL language using DELPHI as development system.

At some times, the text will closely relate to programming features using specific wording related to the computer language. Therefore, it is not required but may be helpful to have some basic understanding in programming.

The code of a (larger) PASCAL program is usually structured in different files called *units*. Modern software development is often using object-oriented programming . Here, an *object* consists of specific data and methods to work with these data. Often, data that are mainly used together (e.g., climate data of a given day) are organised as *records*. Some figures in the document that explain single steps of the data processing contain at the right-hand side marks like //*CDY#03. These marks are also written in the code and can help to find the related code using a search function.

Model description

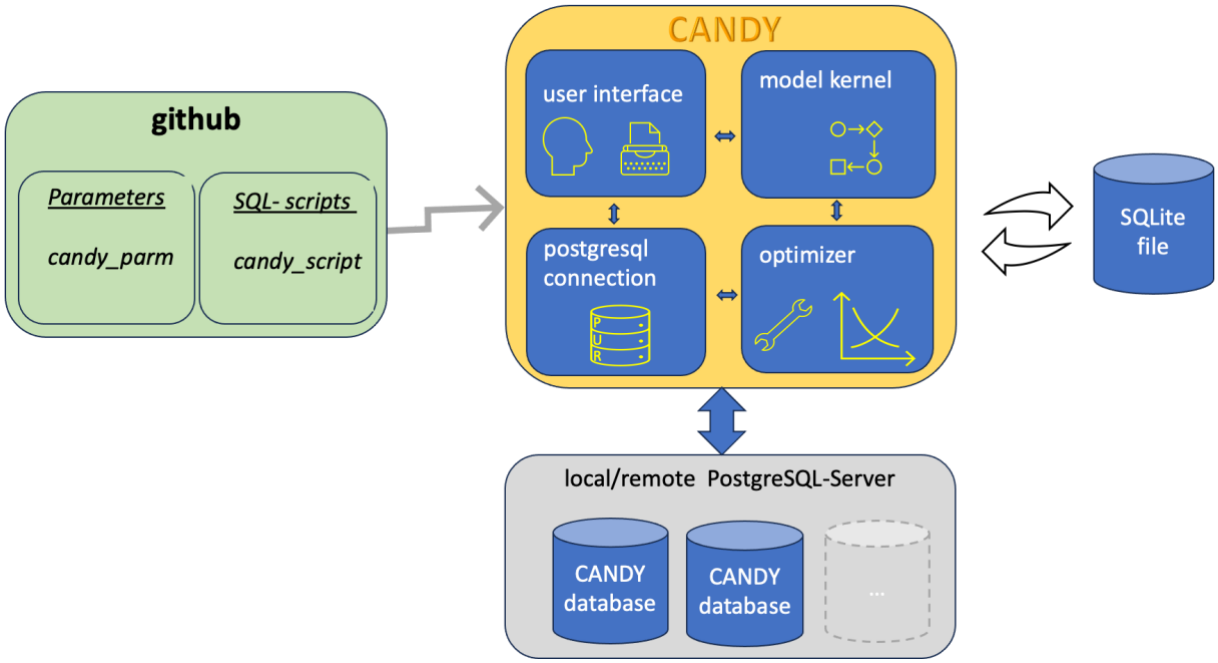


Figure 1: modular construction of the CANDY system

Introduction

The agro-ecosystem model CANDY (Carbon And Nitrogen DYnamics) has been developed to describe carbon and nitrogen dynamics in arable soils and grassland in order to provide information about carbon stocks in soils, organic matter turnover, nitrogen uptake by crops, leaching and losses to atmosphere. A detailed description about using the user interface can be found in the CANDY 22 MANUAL I.

The CANDY model started its history as an integrated simulation tool for carbon and nitrogen dynamics in soils providing a user interface to handle input and output data. During several projects and with the input of many people, more and more adjustments have been made to make the model usable for the specific task. Nowadays we talk about CANDY as a system consisting of several modules where some of them are mandatory for ecosystem modelling because they provide the basic infrastructure, while others may be switched on or off depending on the objective and the available data.

Good modelling practice

It is strongly recommended to start with a critical evaluation of the model and the parameters because some specifics of the site or the management system may lead to different results than expected. In this case a new calibration may be required or some more work is necessary to identify additional processes that are not yet included in the model.

CANDY is a system in continuous development. This means that the reliability of the individual modules may vary over time. Some modules are used with good results over many years, while others may be rather new with only limited research use.

The system provides an infrastructure (Figure 1) of specific modules and a database connection to access model parameters as well as user specific data such as initial soil values, weather data, soil management data and measurement values. CANDY parameters can be updated from a *github* repository, and the included optimiser helps to adapt them to special conditions. Further, a data exchange between several candy users is possible via import and export of SQLite – databases that are condensed in a single file.

Model specific input data comprises soil and plant properties as well as process parameters, scenario related data to describe the agricultural management, climate and observed features.

Th components of the model kernel (Figure 2) describe the dynamics of temperature, water, carbon and nitrogen in relation to crop growth in soil including changes in soil structure.

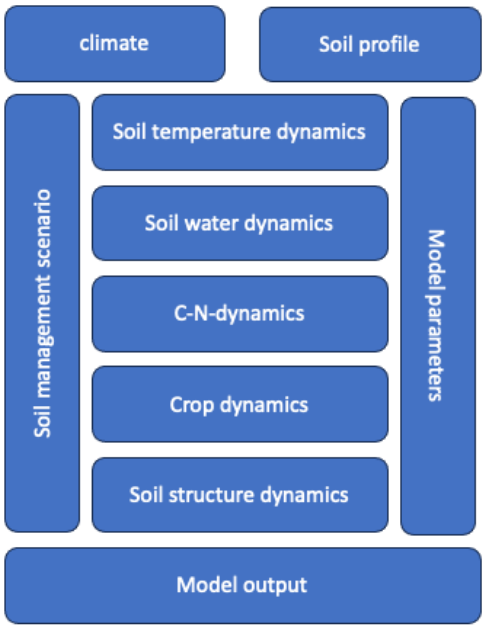


Figure 2: components of the model kernel

The model results consist of soil and crop related state variables and fluxes connected to soil organic matter, nitrogen, and water.

Special features of CANDY are:

- The model calculates a biologic active time (BAT) which allows the assessment of organic matter turnover for different sites and gives the possibility to calculate the steady state of soil organic matter.
- A weather generator provides the possibility to simulate long term scenarios repeating a given crop rotation several times.
- The growth of selected crops (e.g., grassland, maize, wheat ...) can be simulated depending on environmental and agronomic conditions (e. g., weather, soil, fertilisation).

The modules of the CANDY system may use different parameter sets. For example, the user must develop a clear idea about the objective of the modelling work and the required basic data. It is necessary to check the available parameter tables if they contain already the required items.

The CANDY infrastructure covers the main processes that are relevant for an agroecosystem and the required facilities for the data management as mentioned in the following paragraphs.

Access to soil properties

Soils are of central and crucial relevance in CANDY. Each simulation is performed on a specific soil considering a sequence of agricultural activities and a specific weather course. The soil is regarded as a one-dimensional profile consisting of separate horizons that are mainly characterised by soil texture and a set of soil physical properties. In contrast to natural horizon dimensions the model considers the soil profile as sequence of homogenous layers of 1 dm thickness. Depending on the chosen simulation mode, the physical properties can be handled as parameters (constant values over time) or as state variables with an inherent dynamic.

Access to climate data

Climate data are usually available as daily observations, but CANDY can also use a climate generator or aggregated climate values. In any case the climate module delivers daily values to all other sub-models.

Access to management data

This module distributes the management information to the appropriate sub-models. Sometimes this requires some search activities in the data and the breakdown for instance of a slurry amendment into mineral fertilisation, adding of organic matter and water input. Each tillage operation leads to averaging of the state variables of the affected calculation layers.

Access to observation data

All observation data (aka measurement results) are stored within a specific table (*cdy_mvdat*). During the preparation of a simulation run all or selected data are temporarily moved to another table (*cdy_msdat*) that is used by the model. This table may also include data records that are not based on real observations and are only used to get information from the model. After simulations that take very long time, it may be useful to move the result data from the temporary table back into the permanently stored part.

Access to parameter tables

All parameters are accessible over the user interface as described in the CANDY 22 MANUAL I. In some cases (e.g., the soil data), there is a specific interface. In other cases, the data administration requires more knowledge about the data organisation. An additional SQL-module supports users that have no separate software for database management available.

Generation of result records

Beside the interface to the measurements (here mostly referred to as observations), users may select several predefined results (e.g., groundwater recharge, carbon stock, N2O emissions etc.) in an appropriate time resolution (day, … , month, year). This is less flexible, but the preparation is usually easier.

Process modules

The basic process modules are 'soil water dynamics', 'soil temperature dynamics', 'crop development' including permanent grassland and livestock, 'soil organic matter turnover' and 'nitrogen dynamics'. They are all integrated – together with other procedures - in the code unit *cdyspsys*. There are several preparations required before the actual simulation can start and depending on how the model is started there are special workflows to be considered (Figure 3). The model can be started in batch mode from a command line of higher or lower complexity or from the graphical user interface (GUI) for a selected set of plots. Anyway, the workflow comes to the procedure *start_candy* in unit *cdy22_config* that will first create and then initialise the candy kernel with its sub-modules (Figure 5).

Description of the simulation system

The following chapters present the currently available process modules with a focus on the description of the used algorithms.

CANDY is developed as a collection of several connected modules or objects, each relatively independent to solve a specific task. Some objects are related to data flux organisation of e.g., management, climate, observations, and results. Other objects

cover the description of processes in the soil plant system. All objects are characterised by their task, input and output data as well as parameter requirement.
Before the detailed explanation of single components, an overview about the single steps that follow the start-up of the app (Figure 3) with reference to the code units and the main procedures is given. It illustrates how the simulation is started from a batch call or inside the GUI that lead both to the procedure *candy_start* in unit *cdy22_config*.

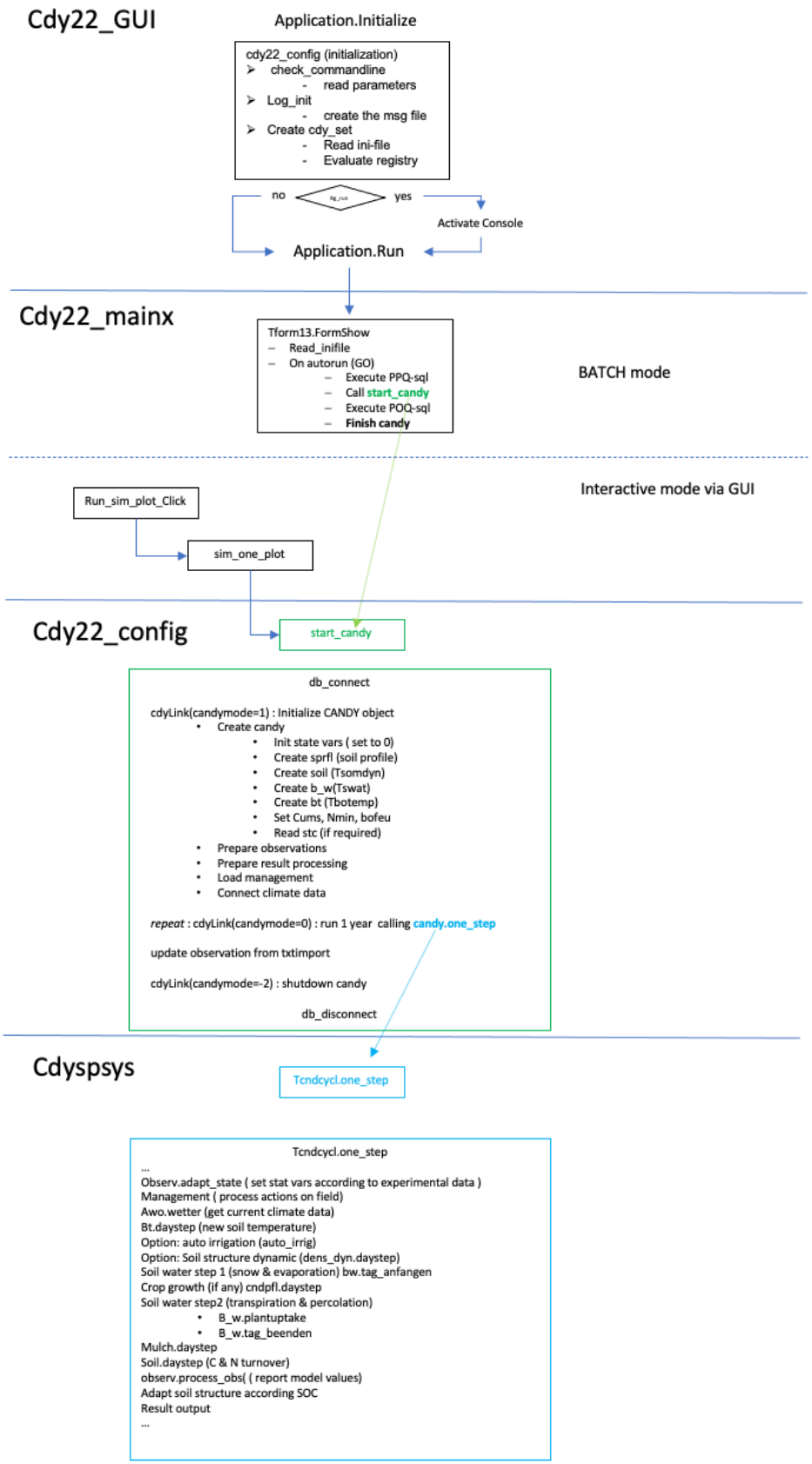


Figure 3: workflow and information flux for a CANDY run (programmers view)

Processing a simulation scenario

Figure 5 illustrates the single steps of a scenario simulation (*sim_one_plot*) starting with the setting of task parameters. Based on the selected plot, the task is characterised by the soil profile, the climate station and the time frame of management data that may be repeated for a given number of cycles (Figure 4). The required climate data will be taken from the database or from the integrated climate generator. The system takes care to use the proper time scale for management as well as for climate and result outputs. The latter can be approached in different ways: Some outputs are written as messages into a text file (*.msg), while results and observation outputs are managed according to the selected lists as defined in tables *cdy_prop_lst* and *cdy_rslt_lst* (see description of output features in the CANDY 22 MANUAL I and chapter Model output) .

After task initialisation, the algorithm conducts a repetitive process chain. Beginning with the basic management interval, all years within that interval are processed one by one, addressing management actions and soil processes for each single day as shown in Figure 6 within the one_step method of the CANDY kernel object. If necessary, a management cycle can be repeated several times with continuous climate data as demonstrated in Figure 4.

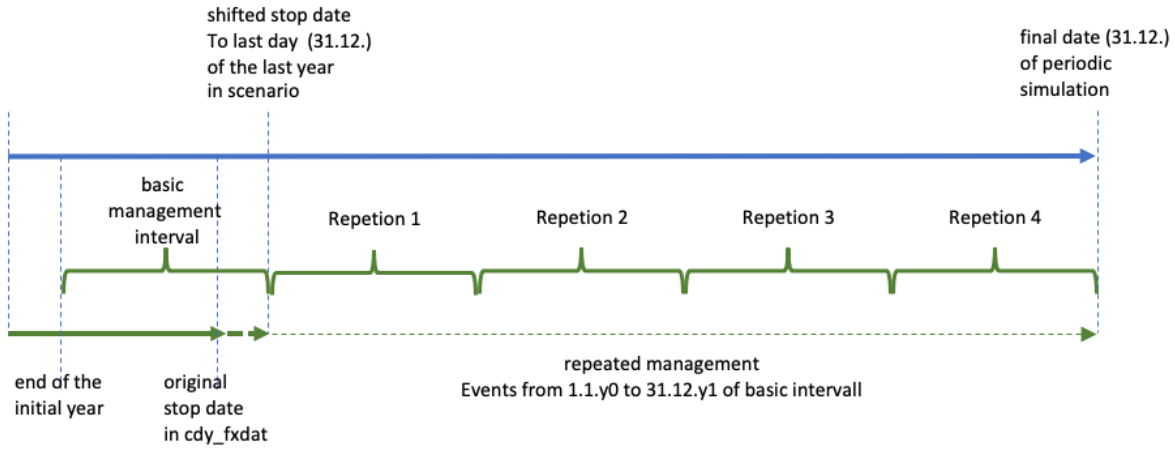


Figure 4: scenario simulation with repeated management cycles

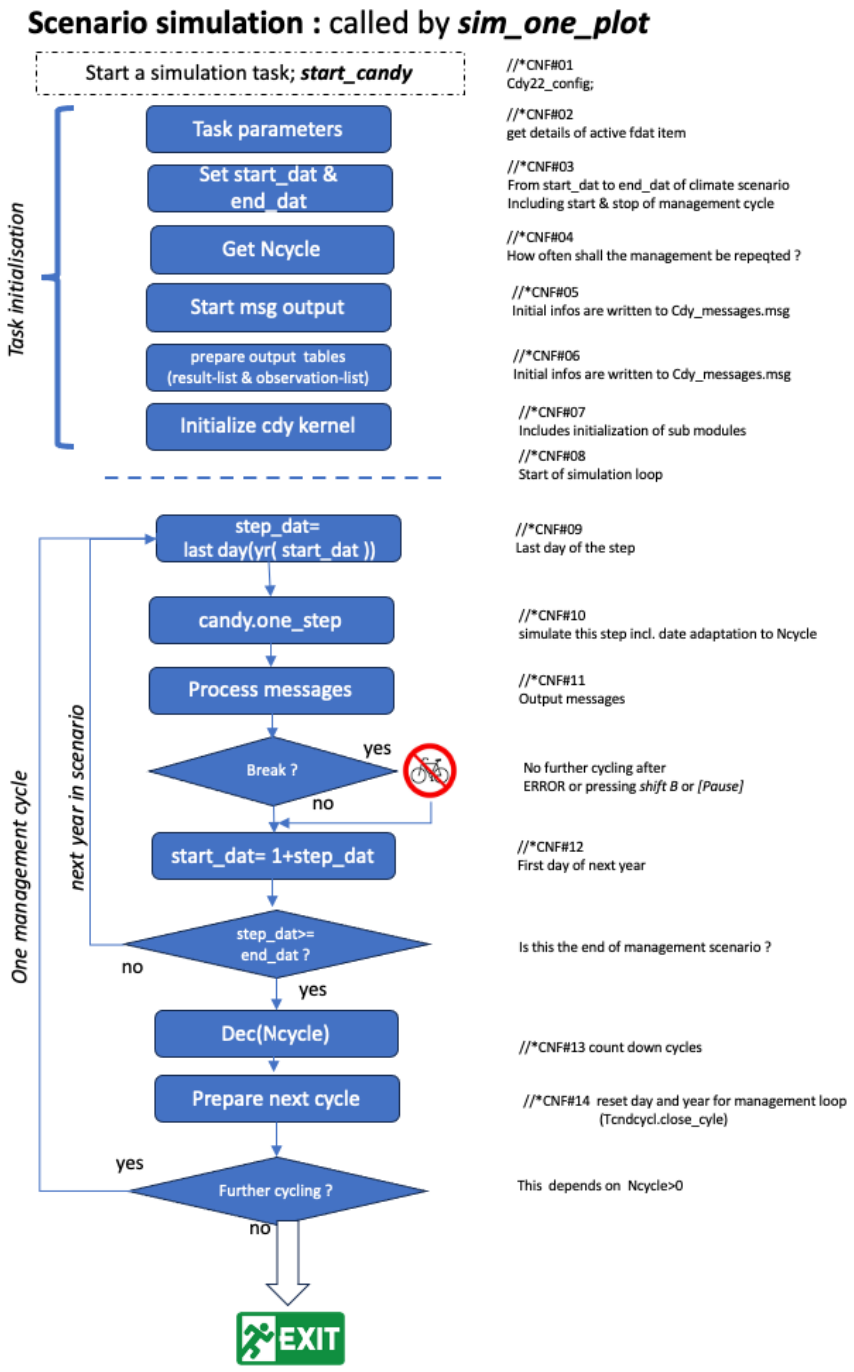


Figure 5 principal steps of a scenario simulation

Sequential call of sub models in candy.one_step

After some more preparation steps, the method candy.one_step is called (Figure 6). It wraps different sub-modules that are called one after another in daily timesteps within a one-year-loop. Within each daily timestep all required sub-models are called as shown in Figure 6. This day-by-day simulation will continue until reaching the specified scenario end-date. The following chapters provide more detailed descriptions of single modules.

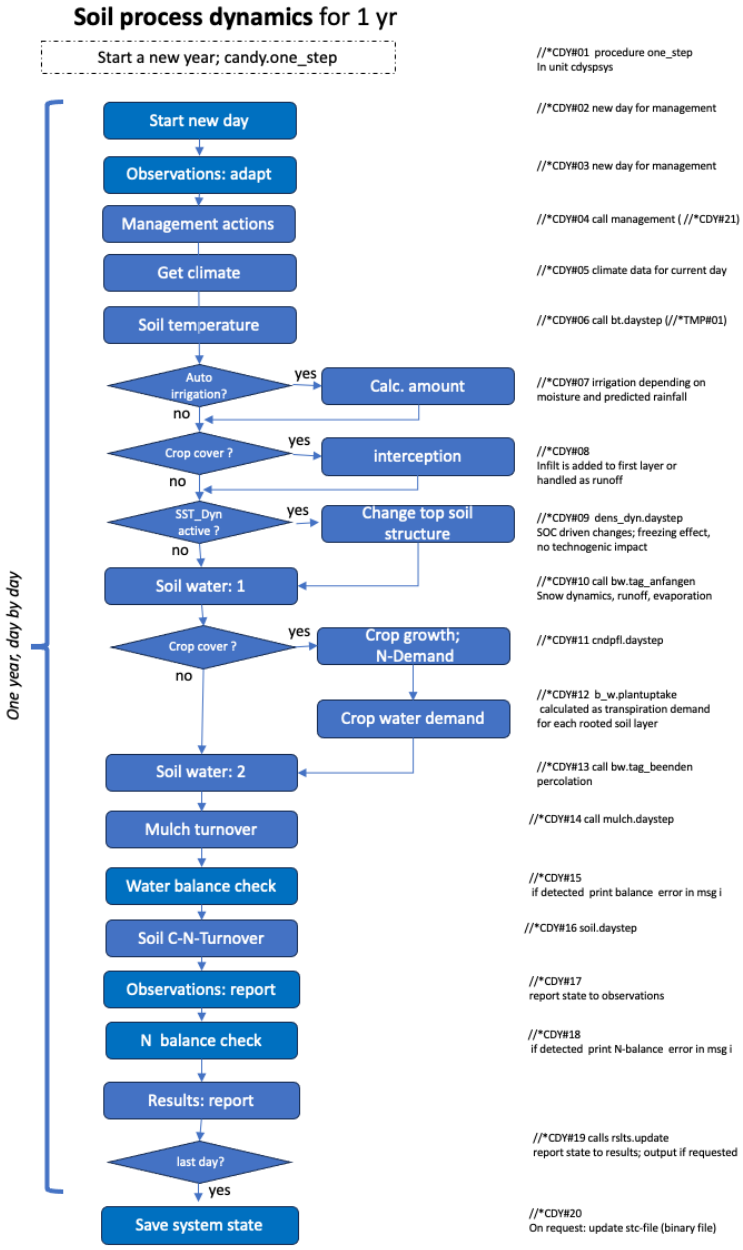


Figure 6 : daystep of a CANDY simulation

Processing observation values (measurements)

The processing of observation data is split into two steps. At the beginning of each daily cycle, CANDY checks the requirement for an adaptation of internal state variables (adapt Y/N) from input values. This is an option to overwrite the initial conditions set by default with values given by the observation data. At the end of the daily cycle CANDY checks what output is required for model evaluation and writes the current values of internal state variables into an output stream that will update the field *s_value* in table *cdy_msdat*. In addition to the *observation* data, which are used to assess model performance and refer to previously freely chosen time and depth

intervals, there is also an output stream via the *result* data. There, the simulated values are condensed to more or less aggregated state variables and written into the result table at previously chosen fixed time intervals.

Processing management activities

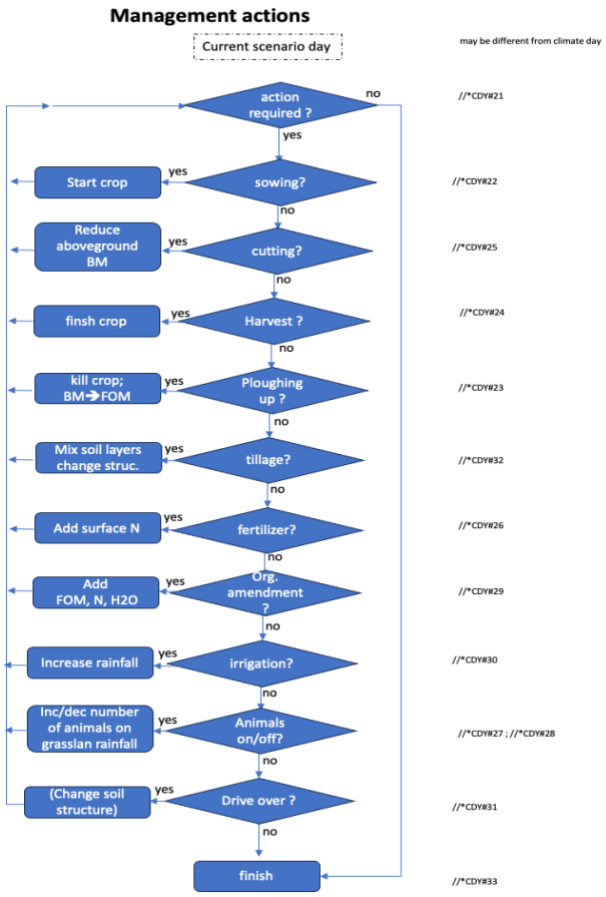


Figure 7: schematic view on the processing of management actions

The management activities are taken from the table *cdy_madat*. If the management cycle has to be repeated, the date in the table is synchronised with the simulation date adapting the year (Figure 7). It is generally taken care that leap years don't disturb the scenario run but avoiding actions on the 29. February may not be the worst idea. The following management activities can be deployed in the model:

Sowing cutting and harvest are processed via the crop model which will be described in a later paragraph.

Ploughing up will stop plant growth, handle the so far existing biomass as organic amendment, and performs a tillage operation.

Tillage leads to a mix (averaging) of all state variables within the addressed soil layers. If the option for soil structure dynamics is activated, it will also change soil bulk density that will lead to further changes of soil physical parameters.

The addition of mineral N *fertiliser* will increase the nitrate and ammonia nitrogen of the first soil layer (0-10 cm) according to the fertiliser properties.

Organic amendments are more complex. The application is broken down to an input of mineral N, water, and pure organic matter.

If an *irrigation* action is detected, the water is simply added to the amount of already corrected rainfall of the given day.

If the plant cover is grassland (handled by the grassland module), it is possible to have *grazing animals*. Their number can be increased or decreased by the appropriate action.

Processing climate data

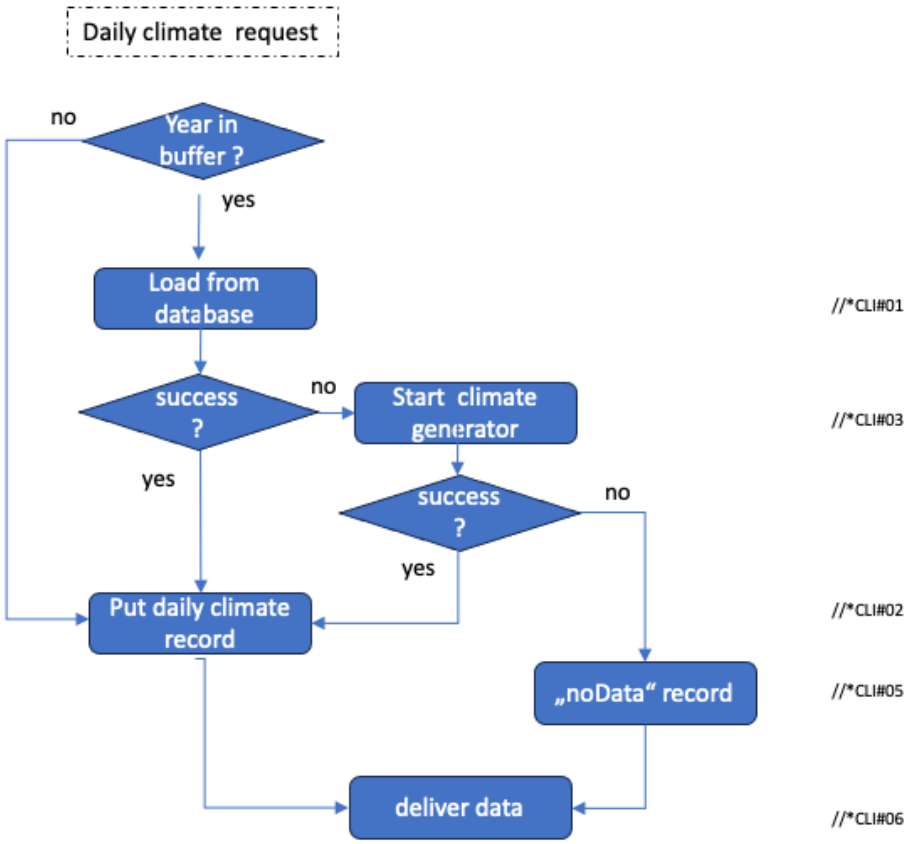


Figure 8: providing daily climate data

The climate object has an internal buffer to store the climate data for one year. Each day, a request for climate data is directed to the climate data object to check whether the year of this date is already in the buffer. If this fails, the buffer is filled with new data from the database. If this is not successful because the data cannot be found in

the database, it is tested whether a climate generator can be started as an alternative. If this also fails because no parameter file is available, the request is answered with an error message.

If the request can be met, the data record is compiled from original data and calculated values and contains:

Real amount of rainfall (nied_k) : Considering that the measurement of rainfall is subject to systematic errors, the original value is adjusted according to the algorithm from Richter (1985) if the daily air temperature is above 0.5 °C and according to Rachner & Matthaeus (1981) if it is below that threshold.

Global radiation (glob): If **no** global radiation was observed, this value is calculated from sunshine duration considering the potential radiation amount for the given day at the location.

Potential Evapotranspiration (pet, pe, pei): These are three classes of atmospheric water demand where the calculation is based on the approaches of Turc (1961) and Koitzsch (1990):

$$\hat{E}_p = 0.0041 \cdot (T_{air} + 22.7) \cdot (G + 2.09)$$

$$E_p = \begin{cases} tb \cdot \hat{E}_p & if\ T_{air} > 0.5 \\ tu \cdot \hat{E}_p & if\ T_{air} \leq 0.5 \end{cases}$$

$$EI_p = \hat{E}_p \cdot 1.3$$

EI_p	potential evaporation of intercepted water by crop	[mm d^{-1}]
E_p	value of pan evaporation	[mm d^{-1}]
T_{air}	air temperature	[°C]
G	daily global radiation	[MJ m^{-2}]

The requested data are provided in the *simwet* record with following standard content:

datum	: string[10];	current date as text
ltem_h	: real;	today air temperature. (all ltem in °C)
ltem_g	: real;	yesterday air temperature
ltem_v	: real;	day before yesterday air temperature
sonn	: real;	sun shine duration in h
glob	: real;	daily sum of radiation energy in MJ/m² (in DB : J/cm²)
nied_k	: real;	daily (internally corrected) rainfall in mm
nied	: real;	daily observed rainfall in mm
nied3d	: real;	rainfall from today plus next two days
rf	: real;	radiation factor for snow evaporation
pet	: real;	potential evapotranspiration in mm
pe	: real;	potential evaporation in mm
pei	: real;	potential evaporation of interception water in mm

This standard content can be extended to following potential element:

btem	: real;	soil temp. in incubation exp. (if candy is used in this way)
theta	: real;	soil moisture in incub. exp. (if candy is used in this way)
inkub	: boolean;	data from incubation experiment
theta_opt	: boolean;	true: soil moisture in incubation exp. always in optimum
ok	: boolean;	true: record is valid
ltmin	: real;	Minimum air temperature /optional
ltmax	: real;	Maximum air temperature /optional
lfeu	: real;	today rel. humidity in %. /optional
wspeed	: real;	winds peed /optional
gwd	: real;	groundwater distance in cm /optional
ncgw	: real;	N-conc of ground water in ppm /optional

Soil temperature dynamics

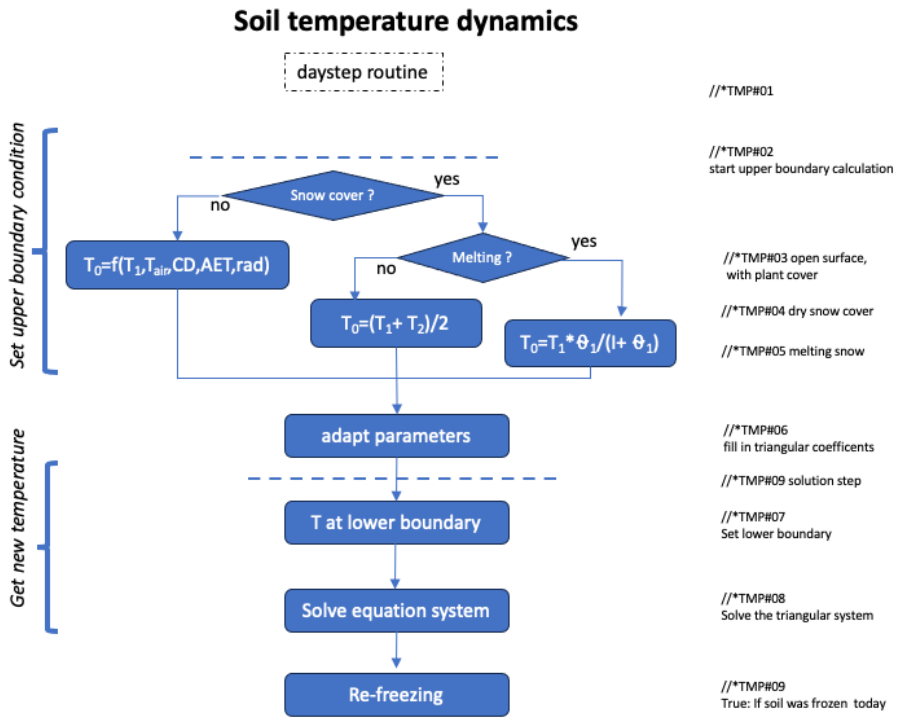


Figure 9: daystep in soil temperature dynamics

Soil temperature plays an important role in many soil processes in the soil, such as chemical reactions and biological interactions. Soil temperature varies in response to exchange processes that primarily take place through the soil surface.

The soil temperature influences the soil water viscosity and thereby the water fluxes within the profile. In the CANDY model, the influence on the C/N turnover is considered through a reduction function during calculating the Biologic Active Time. The daily change of soil temperature for each layer is calculated based upon upper and lower boundary conditions. Several approaches were tested to estimate soil surface temperature. From these experiences is recommended to use the option that is specified in CDYAPARM as BT_MODEL=2.

The simulation of soil temperature in CANDY is encapsulated in one object providing the methods *create* and *daystep*. The *create* routine reads all the necessary parameters on initialisation while the *daystep* routine (Figure 9) is called daily to provide the soil current soil temperatures for each calculation layer.

Input

symbol	**description**	**unit**	**source**
T_{air}	daily mean air temperature	[°C]	CDY_CLDAT
snow	amount of snow	[mm H_2O]	Internal
CC	crop cover degree	[0..1]	Internal
Θ	soil moisture	[mm H_2O]	internal

Output

symbol	**description**	**unit**	**Item_ix**	**Resultnr**
T_s	Soil temperature	[°C]	9	110 (0-3 dm)

Parameters

symbol	**description**	**unit**	**source**
T_{air}	daily mean air temperature	[°C]	CDY_CLDAT
θ	soil moisture	[Vol. %]	Internal
CC	crop cover degree	[0..1]	Internal
snow	amount of snow	[mm H_2O]	internal
$HKAP_d$	specific heat capacity of the dry soil	[J cm^{-3} K^{-1}]	CDY_HRZN
AM_up	amplitude of surface soil temperature	[°C]	CDYBTPRM
PH_up	phase shift of surface soil temperature	[d]	CDYBTPRM
MT_up	mean surface soil temperature	[°C]	CDYBTPRM
AM_lo	amplitude of soil temp. at lower boundary	[°C]	CDYBTPRM
PH_lo	phase shift of soil temp. at lower boundary	[d]	CDYBTPRM
LTEM	mean annual air temperature	[°C]	CDY_FXDAT

Parameters in *italics* are not mandatory. These parameters can be specified for different soil profiles. In this case the table *cdybtprm* needs to have a column named *profil* that is linked to the *profile* table.
Further parameters are shown together with individual equations. Their values are stored in table *cdybtprm*

Description

The state variable of the temperature module is the soil temperature (T_s), which is modelled by solving the heat flow equation after Suckow (1987):

$$\frac{\partial(HKAP_m * T_s)}{\partial t} = \frac{\partial}{\partial z}\left(\alpha * \frac{\partial T_s}{\partial z}\right)$$

t	time	[d]
z	depth	[cm]
$HKAP_m$	specific heat capacity of moist soil	[J g^{-1} K^{-1}]
T_s	soil temperature	[K]
α	actual thermal diffusivity of moist soil	[m^2 s^{-1}]

An upper and lower boundary condition must be determined to solve the equation and get a new temperature profile.

If there is no snow cover, the soil surface temperature ($\hat{T}_0$) as upper boundary condition is calculated from the soil surface temperature of the previous day ($\hat{T}_{-1}$) together with the air temperature (T_{air}), the global radiation (RAD), the crop coverage (CC) of the current day and the evapotranspiration (AET) of the previous day.

$$\hat{T}_0 = F_{ST} * \hat{T}_{-1} + F_{AT} * T_{air} + F_{RA} * \exp(E_{RA} * \ln(RAD)) * \exp(F_{cc} * CC) + F_{ET} * AET$$

Surface temperature is assumed to be equal to the temperature of the first soil layer. at 5 cm depth. The parameters of this equation are taken from table CDYBTPRM for the temperature ranges low ($T_1 < 2$) and high (otherwise).

$\hat{T}_0$	soil surface temperature of today	[°C]
$\hat{T}_{-1}$	soil surface temperature of yesterday	[°C]
T_{air}	daily air temperature (2 m)	[°C]
RAD	daily global radiation	[MJ m^{-2}]
CC	crop cover	[0…1]
AET	evapotranspiration	[mm]
F_x	weighing factor of element x, specified in CDYBTPRM	
E_{RA}	scaling factor for radiation impact, specified in CDYBTPRM	

If the soil is covered by snow, the surface temperature is calculated from the soil temperature of the previous day and the infiltration of melting water that is mixing with the soil water. In case of snow cover and water percolation into the first soil layer the surface temperature is determined by the water amount in soil layer 1 (θ_1) and the infiltrating water (I) assuming the latter has a temperature of 0°C

$$\hat{T}_0 = \hat{T}_{-1} \cdot \frac{\theta_1}{\theta_1 + I}$$

If the snow is not melting i.e., there is no water infiltration, surface temperature is the average of the first two soil layers:
$\hat{T}_0 = 0.5 * (T_1 + T_2)$

A lower boundary condition is assumed at a depth of 200 cm. The soil temperature distribution within the profile is calculated using upper and lower boundary condition. The soil temperature at 200 cm is calculated depending on Julian day

$$T_{lo} = AMP * sin\left((dnr + PHI)^{\frac{2\pi}{365}}\right) + LTEM$$

T_{lo}	daily soil temperature in summertime	[°C]
AMP	Amplitude	[°C]
dnr	Julian day	-
PHI	phase shift	[d]
LTEM	mean annual air temperature	[°C]

Standard values for AMP and PHI are calculated assuming a damping of the sinusoidal surface temperature wave controlled by a help parameter h with

$$h = -z * \sqrt{\frac{\pi}{365 * \alpha}}$$

where

z: soil depth in m

α: average thermal diffusivity of soil profile

The values for AMP and PHI for a given depth z are:

$$AMP_z = AMP_0 * \exp(h)$$

$$PHI_z = PHI_0 + \frac{365 * h}{2\pi}$$

If the surface values for AMP and PHI are not specified in CDYBTPRM for a given soil, default values are used (AMP_0=11, PHI_0=170).

Thermal diffusivity α is based on thermal conductivity and specific heat. Thermal conductivity (λ in $Wm^{-1}K^{-1}$) depends on soil structure as well as on sand and stone content and is calculated as average for the whole soil profile. First, the value for fine soil (λ_s) using the approach of KERSTEN (1949) is calculated:

$$\lambda_s = p_1 * \left(p_2 * lg_{10}(\frac{FC}{BD}) + p_3\right) * 10^{(p_4 * BD)}$$

FC soil moisture at field capacity in VOL%

BD bulk density in g cm^{-3}

The p_i values depend on soil texture and volumetric stone content (stc)

Soil type	p_1	p_2	p_3	p_4
$sand > \frac{1+stc}{2}$	0.1442	0.7	+0.4	0.6243
$sand \leq \frac{1+stc}{2}$	0.1442	0.9	-0.2	0.6243

The effective value for each layer is a weighted average from fine soil and rock (here the value for granite):

$$\lambda = (1 - stc) * \lambda_s + stc * 2.93$$

Next is required the specific heat cv in J/kg/K:

$$cv = \frac{100 * cs + 4190 * \frac{FC}{BD} * (1 - stc)}{100 + \frac{FC}{BD} * (1 - stc)} * BD * 10^3$$

where cs =721.22 is the specific heat of the rock material in J/kg/K

Finally, we get:$\alpha = \frac{\lambda}{cv}$

To improve the fit of simulated to measured data, the parameters AM_lo, AM_up, PH_lo, PH_up and MT_up (table *cdybtprm*) can be calibrated to the temperature curve of several years (Figure 10).

Standard values for the parameters are:

AM_up: 9.5 , PH_up=185 , and MT_up is taken from the *cdy_fxdat* table

AM_lo and PH_lo will be determined as shown above.

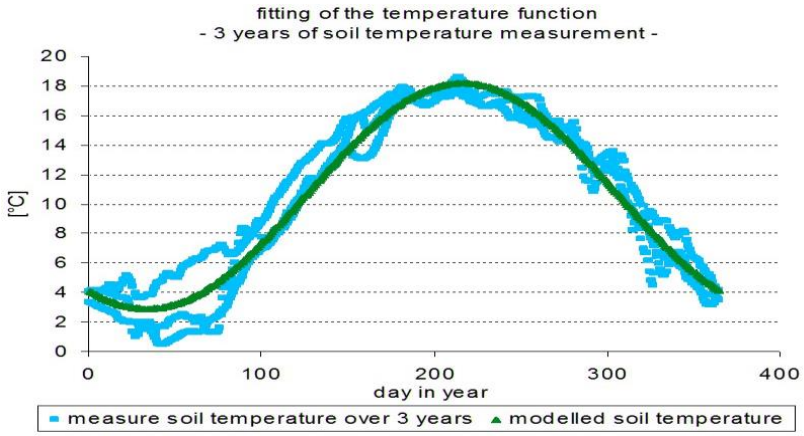


Figure 10: fitted soil temperature function to observed data over 3 years

References

https://www.methodenwiki-bodenkunde.de/MethodenWiki/AGBoden:Verknüpfungsregel_1.32

KERSTEN, M.S. (1949): Thermal Properties of Soils. – Bulletins Institute of Technology, Engn. Exp. Stat., Bull. No. 28; University of Minnesota.

Soil water dynamics

The description of soil water dynamics is distributed amongst different procedures within the cdy kernel(one_step), the soil water object, and the plant object.

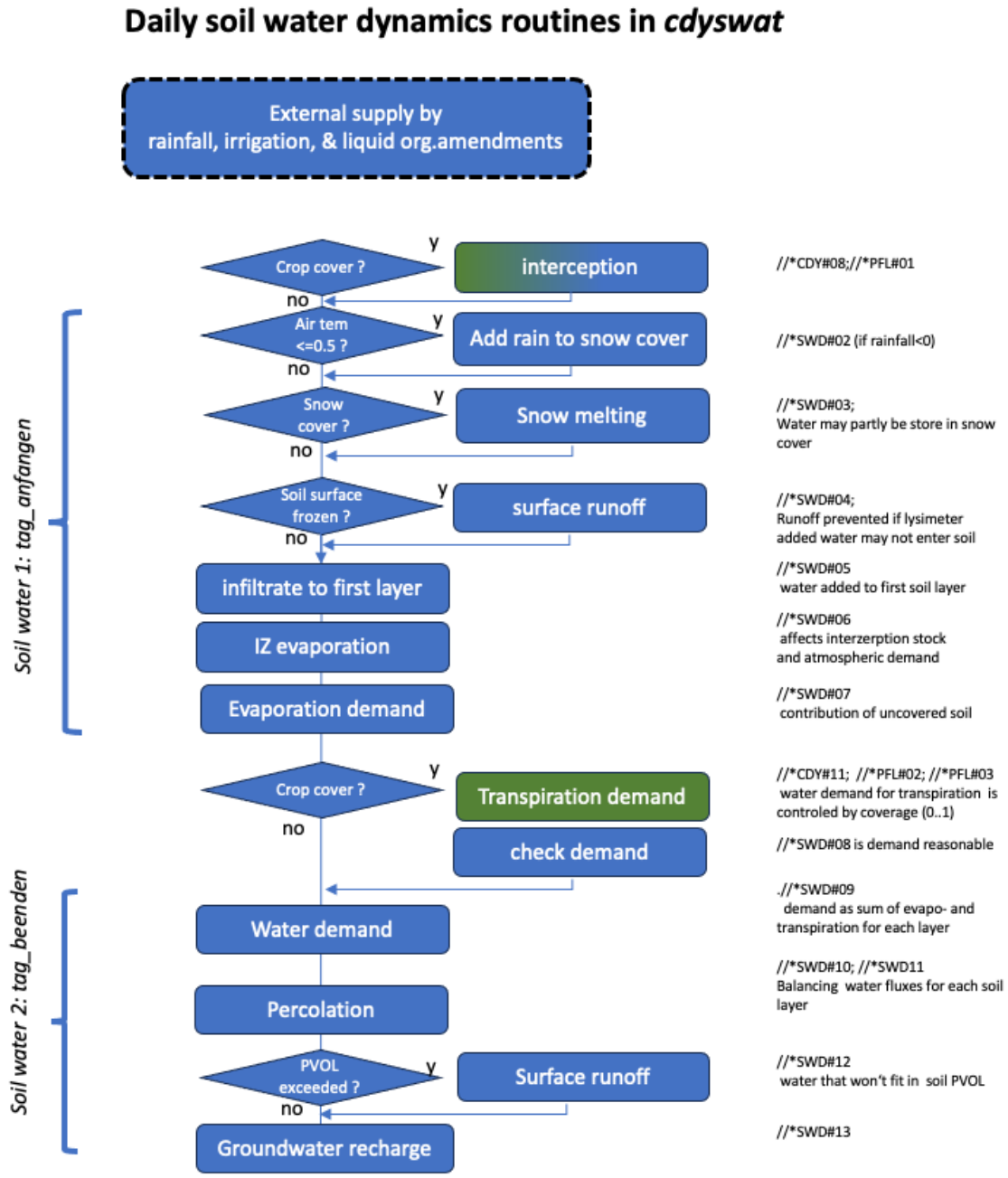


Figure 11: daystep in soil water dynamics

Input

symbol	description	unit	source
P	daily precipitation	[mm]	CDY_CLDAT
T_{air}	daily mean air temperature	[°C]	CDY_CLDAT
G	transformed daily global radiation from J cm^{-2} into MJ m^{-2}	[MJ m^{-2}]	CDY_CLDAT
CC	CropCover: soil surface fraction covered by plants	[0…1]	Internal
h_{pl}	Plant or crop height	[cm]	Internal

Output

symbol	description	unit	m_ix	resultnr
θ	water content of a soil layer	[mm]	10 (Vol%)	108 (0-3 dm)
			11 (M%)	115 (profile)
GW_seep	Seepage to groundwater	[mm d^{-1}]	24	103
ET_p	potential evapotranspiration	[mm d^{-1}]	47	158
ET_a	actual evapotranspiration	[mm d^{-1}]	53	142
Wflux_lay	Water flux from soil layer	[mm d^{-1}]	54	-
WSAS	Water storage above soil	[mm]	-	140

Parameters

symbol	description	unit	source
CZEP	Crop specific interception capacity	[mm cm^{-1}]	CDYCROPS
λ_p	drainage parameter	[mm^{-1} d^{-1}]	Internal
K_s	saturated hydraulic conductivity	[mm d^{-1}]	CDY_HRZN
PV	Pore volume	[Vol. %]	CDY_HRZN
FC	water content at field capacity	[Vol. %]	CDY_HRZN
PWP	permanent wilting point	[Vol. %]	CDY_HRZN
FAT	clay and fine silt (particles ≤ 6.3 µm)	[M. %]	Internal
ABT	elutriable particles < 20 µm	[M. %]	Internal

Description

The state of soil water is described in terms of the amount of water and the energy associated with the forces that hold the water in the soil. The amount of water is defined by the water content. The energy state of the water is given by the water potential. Plant growth, soil temperature, chemical transport, and ground water recharge are all dependent on the state of water in the soil. While there is a unique relationship between water content and water potential for a particular soil, these physical properties describe the state of the soil water in distinctly different manners.

Water flux—the movement of water—occurs within the soil profile, between the soil and plant roots, and between the soil and the atmosphere. As in every natural system, movement of a material is dependent on energy gradients. The fundamental forces acting on soil water are gravitational, matric, and osmotic. Water molecules have energy by virtue of position in the gravitational force field just as all matter has potential energy. This energy component is described by the gravitational potential component of the total water potential. The influence of gravitational potential is easily seen when attractive forces between the water and the soil are less than the gravitational forces acting on the water molecule and water moves downward. The arrangement of soil solid particles determines the matric potential, often characterised by its logarithmic value *pF*. The magnitude of the forces depends on the texture and the physical- chemical properties of the soil solid matter. Most methods for measuring soil water potential are sensitive only to the matric potential. There is a unique relationship (soil water retention curve) between the water content and the water potential for each soil (Figure 12).

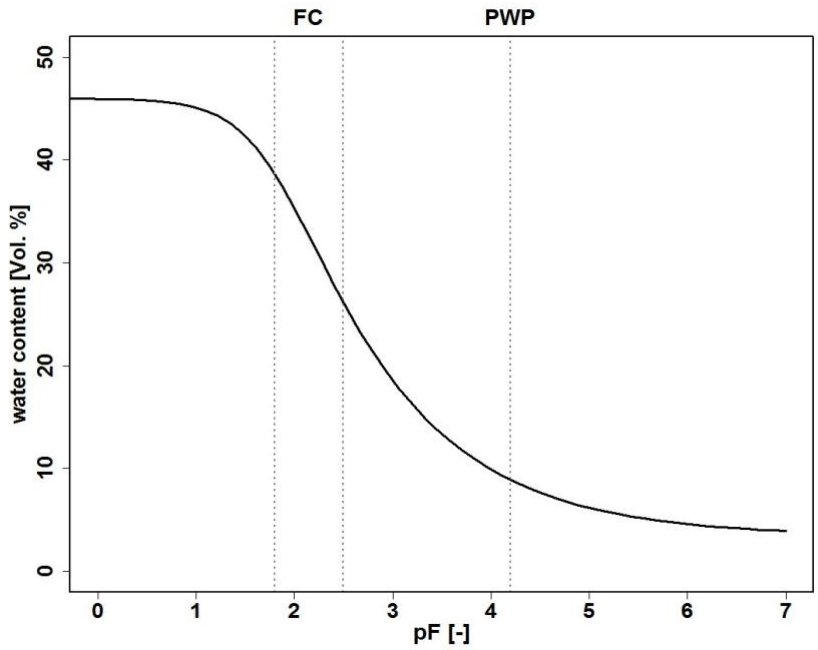


Figure 12: water content dependencies from logarithmic matric potential (pF). (silt soil example)

The CANDY water module describes the relevant processes of water flux in the unsaturated zone (Figure 13) of soils using calculation layers of 10 cm depth. CANDY is a 1-dimensional model, so lateral fluxes are not considered. Surface runoff occurs due to infiltration surplus if the precipitation water cannot longer enter the pore system of the soil.

The CANDY model uses the capacity concept for calculating water flux in the soil/water movement. Downward flow of infiltrated water is only allowed if the water storage exceeds the field capacity (Figure 14).

Initial conditions can be defined by the user via the model interface for each layer by observation data or for the entire soil profile as a given percentage of the field capacity.

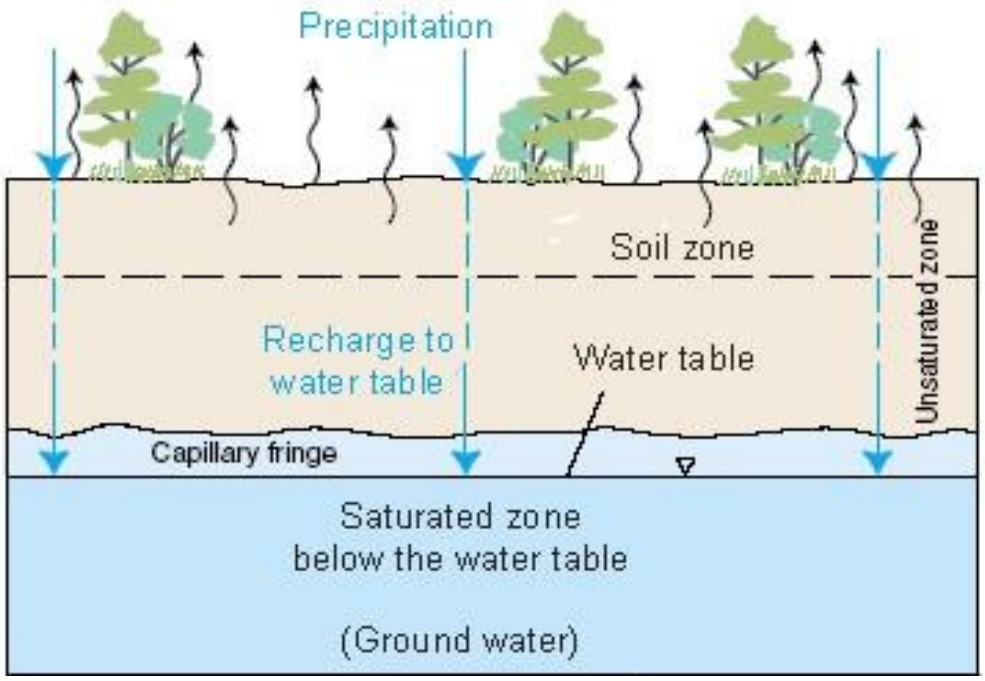


Figure 13: water flux in the unsaturated zone as described by CANDY (http://water.usgs.gov/edu/watercycleinfiltration.html)

Soil specific parameters of the water module can be defined within the soil profile description (tables *profile* and *cdy_hrzn*).

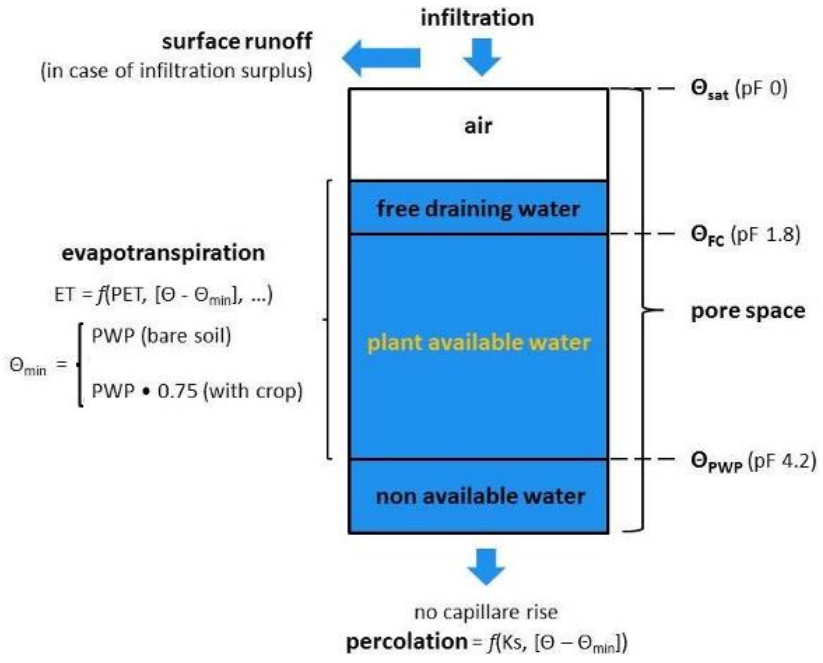


Figure 14: CANDY soil water dynamics for one layer of defined thickness

Water supply and demand

The amount of water that could be added to the soil is mainly coming from the climate sub model given by the daily rainfall but includes also irrigation amount and water added to the soil from organic amendments (like slurry). Also, from the climate sub model comes the information about the atmospheric water demand in terms of potential evapotranspiration which is expressed as a tuple of PE, PEI and PET where each value relates to a specific sub process.

ET_p	potential evapotranspiration PET	[mm d^{-1}]
h	crop height	[cm]
E_p	value of pan evaporation	[mm d^{-1}]
with:	$E_p = 0.0041 \cdot (T_{air} + 22.7) \cdot (G + 2.09)$	
	T_{air} air temperature	[°C]
	G daily global radiation	[MJ m^{-2}]

$EI_p = 1.3 \cdot E_p$

EI_p	potential evaporation of intercepted water by crop	[mm d^{-1}]

PET is adapted to crop height h :$ET_p = (1 + 0.004 \cdot h) \cdot E_p$; $h \leq 100$

Interception

The interception submodule is based on a published approach Koitzsch (1990), Koitzsch and Günther (1990).

Interception is considered if the amount of rainfall is above 0.01 mm and daily air temperature is above 0.5 °C for a soil that is at least partly covered with crops.

The change of interception water is calculated within the crop module. The maximum interception of water by a crop (*ICAP*) depends on crop specific interception capacity (*SCAP*), crop height (h_{crop}) and the fraction of the soil surface covered by the crop (*CC*).

$$ICAP = SCAP * CC * \min(100, h_{crop})$$

The maximum amount that can be added to the interception storage is:

$$\Delta I_{max} = ICAP - AI$$

The potential amount of added interception water depends on rainfall (P) and crop cover (CC):

$$\Delta I_{pot} = P * CC$$

The actual amount of added interception water is given by

$$\Delta I = \begin{cases} \Delta I_{pot}\,;\ \Delta I_{max} > \Delta I_{pot} \\ \Delta I_{max}\,;\ \Delta I_{max} \leq \Delta I_{pot} \end{cases}$$

$$P_{eff} = P - \Delta I$$

The daily added interception amount ΔI fills up the interception store but 50% of the new interception amount is evaporated immediately.

$$AI_{new} = 0.5 * (AI_{old} + \Delta I)$$

$$E_i = 0.5 * (AI_{old} + \Delta I)$$

ICAP	interception capacity	[mm]
AI	Actual interception storage	[mm]
E_i	Evaporation from interception water	[mm]
h_{crop}	crop height	[cm]
CC	CropCover; fraction of the soil surface covered by plants	[0…1]

In case of ploughing up, the interception water is added to soil and *AI* is set to zero.

Snow accumulation and melting

The process of snow accumulation and melting is calculated according to Koitzsch (1990): snowfall is only possible if rainfall occurs, and the mean daily temperature is ≤ 0.5 °C. In this case precipitation is added to the state variable *SNOW*. In case of existing snow cover it will evaporate according to daily PE which is in this case same as PET.

Melting and infiltration can occur if the mean daily temperature > 0.5 °C. In this case the model considers evaporation or condensation depending on daily air temperature. A snow cover can have a capacity to store liquid water (SSC). The SSC value must be set as a batch call parameter (SSC=x) otherwise it is set to zero. Melting depends on daily air temperature and rainfall. The amount of melted snow is first stored as liquid water within the snow cover until the capacity for this storage is exceeded and liquid water is added to the first soil layer. This is not possible in case of frozen soil. If the soil temperature of the first layer is <-0.5 the liquid water is treated as surface runoff. Only if a lysimeter condition is set the water is kept completely on the soil surface.

Evaporation from interception

Water that is stored above ground on plant surface, the interception storage, is easily evaporated. The potential evaporation of interception water, PEI, is calculated in the weather module. If the interception storage is sufficiently filled, the PEI amount is fully evaporated (AE) other ways AE is limited to AI. The further demand for evapotranspiration (PET) is reduced according to:

$$PET_{new} = \left(1 - \frac{AE}{PEI}\right) * PET_{old}$$

Evapotranspiration (soil)

Evapotranspiration in the CANDY water module is allowed if water storage exceeds a soil and horizon specific value of the minimum water content (Figure 14). The process of evaporation is limited to N topsoil layers and calculated depending on potential evaporation PE for the part of soil that is not covered by crops. The value of N is specified as NUNB in table *cdyaparm*. Standard value is NUNB=4.

Transpiration demand

Like evaporation and based on the climatic parameters of the given day given as PET_{new} and the water storage in the rooted, crop covered soil is here calculated how much water can be returned to the atmosphere.

The calculation of water evaporation and transpiration from the soil is based on the work of Koitzsch and Günther (Koitzsch 1990, Koitzsch and Günther 1990). Until this point only the demand for water offtake from each soil layer is calculated. The water uptake by crops is also used to calculate the N uptake by plants.

Crop water uptake

This step is embedded in the percolation routine and finally reduces the water stored in soil layers.

The calculation of actual evapotranspiration is according to Koitzsch (1990). It is based on a maximum demand of water that can be extracted from soil. This demand is reduced, if soil water is not easily available. Furthermore, the total demand is distributed between the soil layers (upper five layers for evaporation; all rooted layers for transpiration) according to the water availability in each layer. Different to more physical oriented models that are based on Darcy's approach and describe the availability with the water potential, the implemented approach in CANDY is assessing the availability in relation to the maximum and minimum water content that are related to field capacity and permanent wilting point. The minimum water amount that has be kept in the soil layer is $\theta_{min} = PWP * k$ with k=0.75 for the first four layers in crop covered soil and otherwise k=1. The maximum extractable water amount of each soil layer is $\theta_{max} = \theta - \theta_{min}$.

$\xi_a = \frac{\xi * \theta_{FC} - \theta_{min}}{\theta_{FC} - \theta_{min}}$ where ξ is taken from XSI in table *cdyaparm*

A weighing factor r is calculated based on a critical water content θ_c and the total daily demand d

$$\theta_c = \begin{cases} \theta_{FC} - \theta_{min}\,; & for\ bare\ soil\ or\ covered\ soil\ with\ d < 2.5\ mm \\ (\theta_{FC} - \theta_{min}) * \left(\xi_a + \frac{1-\xi_a}{17.5} * (demand - 2.5)\right); & for\ covered\ soil\ with\ d < 20 \end{cases}$$

$$r = \begin{cases} \frac{\theta_{max}}{\theta_c};\ if\ \ (\theta_c > 0)\ and\ (\theta_{max} < \theta_c) \\ 0\ \ ;if\ \theta_{max} > \theta_c \end{cases}$$

Which is later used to reduce the water offtake from specific soil layers.

$$ET_a = 0.5 \cdot min(EI_p, R_i) + \Psi \cdot H_1 \cdot max\left(0, \left(1 - \frac{R_i}{EI_p}\right) \cdot ET_p\right) + (1 - \Psi) \cdot H_2 \cdot E_p$$

ET_a	actual evapotranspiration	[mm d^{-1}]
R_i	intercepted water	[mm d^{-1}]
Ψ	fraction of the soil surface covered by transpiring plants	
H_1, H_2	reduction coefficients calculated as function of water content	
ET_p	potential evapotranspiration	[mm d^{-1}]
EI_p	potential evaporation of intercepted water by crop	[mm d^{-1}]
Ep	value of pan evaporation	[mm d^{-1}]

Surface runoff

If the water storage exceeds the pore volume of a calculation layer the amount of the surplus water is added to the calculation layer above. If the soil surface is reached and the puddle storage capacity is exceeded the soil water is considered as runoff. The maximum water storage on the soil surface (*SRF_WC*) must be specified as a batch call parameter in mm. The default value is *SRF_WC=5*. The ability to store a given amount of water on the soil surface must be switched on in the general section of the ini file (*puddle=1*).

Percolation and drainage

The velocity of the downward flow is controlled by the saturated hydraulic conductivity through the drainage parameter (λ_p) (Glugla 1969, Koitzsch 1990). If the actual water content is lower than the field capacity FC, no percolation is possible. The drainage (Q) of each soil layer is calculated by:

$$\frac{d\theta}{dt} = Q = \lambda_p * \frac{(\theta - FC)^2}{[1 + \lambda_p * (\theta - FC)]}$$

Q	Drainage	[mm]

ϴ	water content of a soil column of defined thickness	[mm]
FC	water content at field capacity	[mm]
λ_p	drainage parameter	[mm^{-1} d^{-1}]

The drainage parameter (λ) is internally calculated from the saturated conductivity:

$$\lambda = \frac{0.01 \cdot K_s}{PV - FC}$$

PV	pore volume	[mm]
FC	water content at field capacity	[mm]
λ	drainage parameter	[mm^{-1} d^{-1}]
Ks	saturated conductivity	[mm d^{-1}]

If there are no observation results from water content parameters available, the drainage parameter (λ) or the saturated conductivity (K_s) can be calculated from the elutriable soil fraction (ABT):

$$\lambda = 1.6 - 0.1565 \cdot ABT + 8.424 \cdot 10^{-3} \cdot ABT^2 - 2.551 \cdot 10^{-4} \cdot ABT^3 + 4.28 \cdot 10^{-6} \cdot ABT^4 - 3.625 \cdot 10^{-8} \cdot ABT^5 + 1.207 \cdot 10^{-10} \cdot ABT^6$$

with: $ABT = T + fU + mU$

ABT	elutriable particles < 20 µm	[M. %]
T	clay (< 2 µm)	[M. %]
fU	fine silt (2 – 6.3 µm)	[M. %]
mU	medium silt (6.3 – 20 µm)	[M. %]
λ	drainage parameter after *Glugla*	[mm^{-1} d^{-1}]

Crop module

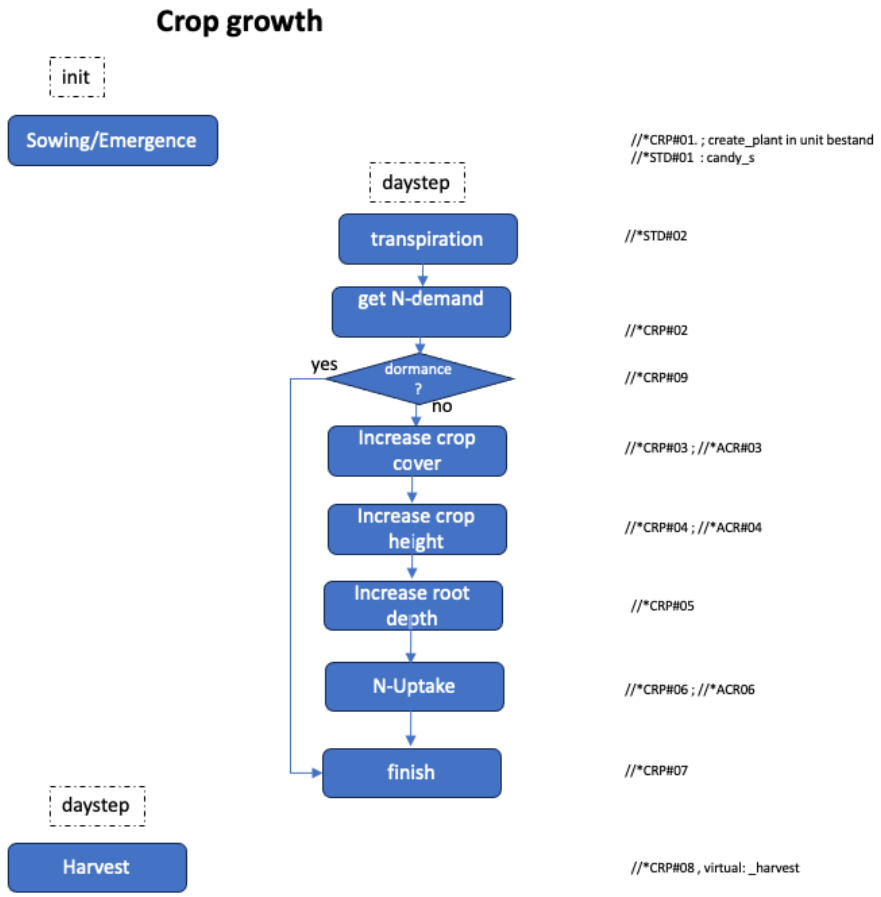


Figure 15: general daystep in crop module

Available plant modules are listed in the following table:

label	modul	comment	ID	create	n_dem.	n_upt	harv.
CANDY_S	stdpfl, Basic approach	Fixed N-uptake for each crop type	0; 1	STD#01	STD#02	CRP#06	STD#03
CANDY_T	trkpfl	N-uptake driven by transpiration	2	TRK#01	TRK#02	CRP#06	TRK#03
ZALF_ZF	zalf zf	Predicts biomass, for catch crops only	4	ZFZ#01	ZFZ#02	CRP#06	ZFZ#03
CDYDGRN	grass, trkpfl descend.	Grazing is included	90	DGR#01	TRK#02	CRP#06	-
AGRO1	autocrop	Generic plant develop-ment model	91	ACR#01	ACR#02	ACR#06	ACR#08

The selection of plant modules in CANDY is enabled by the hierarchical principle in the model structure. I.e., the crop state is always represented by four crop variables

(crop height, root depth, soil coverage, N uptake) independent of the internal complexity of the selected plant module. The plant modules, CANDY_S and CDYDGRN, will be described in the following. All plant modules are descendants from a basic class and are addressed from the main simulation cycle via following routines:

CANDY_S approach for N uptake

Input

symbol	description	unit	source
WERT1	Crop ID	[-]	*cdy_madat*
DATUM	date of sowing	[-]	*cdy_madat* (macode = 12)
	date of emergence, no impact if sowing date was given	[-]	*cdy_madat* (macode = 1)
	date of harvest	[-]	*cdy_madat* (macode = 2; 9)
WERT2	Yield of main product	[dt ha^{-1}] (1dt=100kg)	*cdy_madat*
ORIGWERT	nitrogen uptake	[kg ha^{-1}]	*cdy_madat*

Output

symbol	description	unit	measurement id	result id
N_{upt}	nitrogen uptake	[kg ha^{-1}]	20 (total above ground)	202 (sum)
			56 (per layer)	122 (flux)
CC	crop cover	[0…1	46	127
D	current root depth	[dm]	45	-

Parameters from table cdycrops

symbol	description	unit
item_ix	Internal Crop ID	[-]
name	Crop name	[-]
type	1= summer crop; 2= winter crop 3= annual legume crop ; 4= perennial legume crop 5= perennial crop; 6= grassland with auto-cut	[-]
model	model algorithm, CANDY_S , AGRO1 or CDYDGRN	[-]
transk	transpiration coefficient (max. value in grassland model)	[-]
algo	characteristic of plant (annual (1), bi-annual (2) or perennial crop(3) ;algo=4 means perm. grassland with auto-fertilization	[-]
slope (S)	slope parameter for S curve (N uptake)	[-]
t_veg (V)	days from emergence to harvest	[d]
lnutop	N_{min} uptake rate of legumes from soil	[0…1]
lndsub	part of N stored in subsoil	[0…1]
rdmax	maximum root depth	[dm]
rg10	days for 10 cm root depth growth	[d]

dchmax	days from emergence to maximum crop height	[d]
chmax	maximum crop height	[cm]
matstart	days from starting maturity to ripeness	[d]
ccmax	maximum crop coverage	[0…1]
dccmax	days from emergence to maximum crop coverage	[d]
czep	specific interception capacity related to plant height	[mm cm^{-1}]
zetb	parameter of water withdrawal function	[-]
tk_min	Minimal value for transpiration coefficient	
ts1	Temperature sum	
ts2	Temperature sum	
n_agbm	N content in aboveground biomass (yield + by-product)	[%]
dm_nat	Standard DM of harvest product	[%]
rix	Parameter to calculate stubble mass	[kg/dt]
fix_r	Parameter to calculate root mass	[kg/ha]
stix	Parameter to calculate stubble mass	[-]
fix_s	Parameter to calculate stubble mass	[kg/ha]
bix	Parameter to calculate plant residues	[kg/dt]
sba_id	pointer to a record in SBACROP to characterise crop for automatic fertilization	[-]
rt_ix	pointer to a record in CDYOPSPA to characterise root material	
gm_ix	pointer to a record in CDYOPSPA to characterise aboveground biomass after ploughing up	[-]
sh_ix	pointer to a record in CDYOPSPA to characterise shoot material	
source	data provenience	

Description

"CANDY_S" is an empirical plant module, which describes plant growth and crop development as a sink of soil water and nitrogen. The nitrogen uptake of crops is expressed by a "S-shaped" function depending on the expected N uptake (Figure 16).

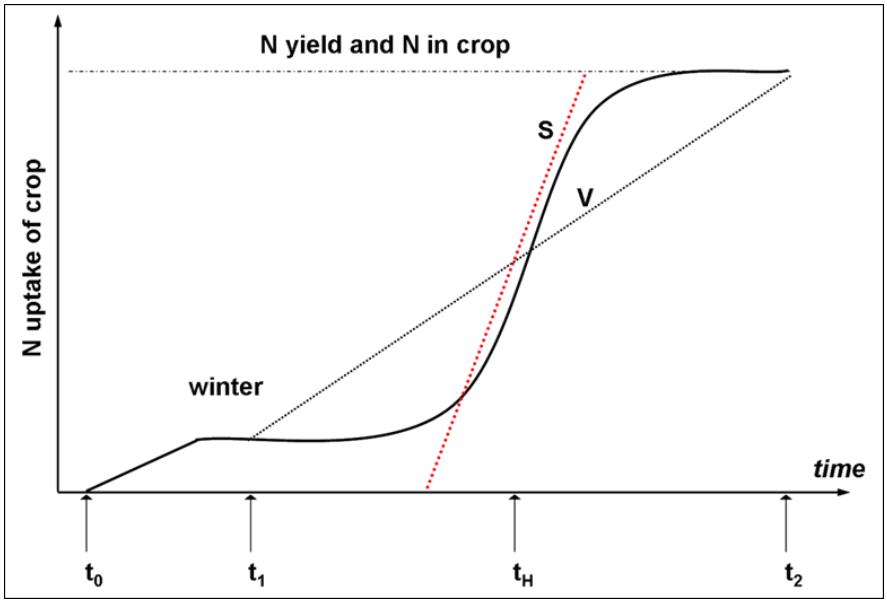


*Figure 16: Definition of the N uptake at crop emergence (t0), start (t1) and end (t2) of the vegetation period (V = crop parameter t_veg) in the harvest year and the inflexion point (tH = (t2 - t1)*0.5). (S = crop parameter slope)*

The mathematical formulation is given by Franko et al. (1995):

$$N_{upt}(t) = 0.5 \cdot \left(1 + \frac{tanh\left(\frac{2 \cdot t}{V - 1}\right) \cdot S}{tanh(S)}\right) \cdot N_{total}$$

N_{upt}	total nitrogen in crop at time t	[kg N ha^{-1}]
t	time (with zero at the begin of plant uptake)	[d]
V	crop-specific duration of vegetation period in harvest year	[d]
S	slope of curve at time t_H	[-]
N_{total}	planned total nitrogen uptake at harvest (intention)	[kg N ha^{-1}]

During the growing season, the nitrogen uptake is possible when plant roots are apparent in a calculation layer. The rooting depth is increased daily according to a linear model of RDMAX (crop specific maximum rooting depth) and RG10 (days for 10 cm root growth) until the RDMAX value is reached. Later, rooting depth remains constant until harvest. If soil moisture reaches permanent wilting point (PWP), the N uptake of the plant is stopped.

A part of the total N uptake returns to the soil as organic matter from harvest residues and roots. The crop related dry matter input is calculated as linear relation depending on dry matter yield of the main product (MP_{dm}) as belowground deposition from roots (RT_{dm}) and aboveground deposition from stubble (ST_{dm}).

$$RT_{dm} = FIX_r + BIX \cdot MP_{dm}$$

$$ST_{dm} = FIX_s + RIX \cdot STIX \cdot MP_{dm}$$

$$BP_{dm} = RIX \cdot MP_{dm} - ST_{dm}$$

with RT_{dm}: amount of root dry matter

ST_{dm} : dry matter amount of stubble

BP_{dm} : dry matter amount of by-product (e.g., straw)

MP_{dm}: dry matter yield of main product

FIX_r: yield-independent part of root dry matter

FIX_s: yield-independent part of stubble dry matter

BIX: belowground index. Yield-dependent part of root dry matter

STIX: stubble index. Relation between stubble and total aboveground residues

RIX: residue index. Relation between aboveground residues to main product

The plant development parameters (crop height CH and crop coverage CC) are calculated as interpolation of days from emergence to time of maximum development (DCCMAX and DCHMAX) and their maximum values (CHMAX and CCMAX) (Figure 17). Additionally, the coverage is influenced by the senescence of the crop. Plant development is considered as independent from nitrogen uptake. The parameter MATSTART determines the number of days from maturity to harvest. During this period, the coverage is reduced continuously. In general, the influence of coverage for the soil temperature is considered..

Since the state variables plant height, coverage, rooting depth, and N uptake are described by empirical approaches as a function of time, they do not depend on environmental influences.

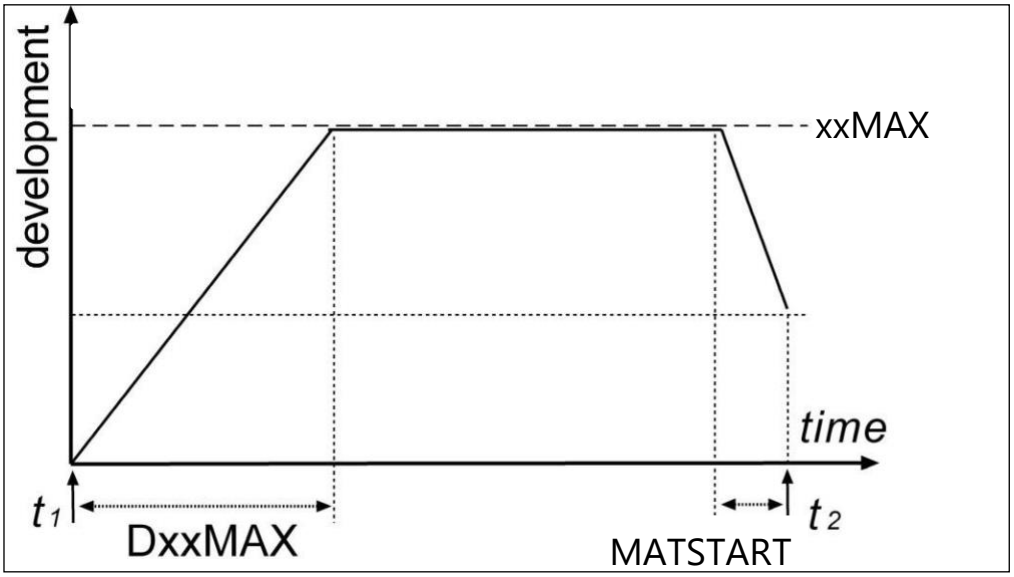


Figure 17: Development of rooting depth, crop height and coverage with xxMAX: RDMAX (maximum rooting depth), CHMAX (maximum vrop height), CCMAX (maximum crop coverage) and MATSTART (days of senescence) as plant parameters within the table CDYCROPS as interpolation of days between start (t1) and end (t2) of the vegetation period.

Legumes

Description

The principle of CANDY_S represents the base for the modelling of legumes and grassland as well. Further parameters complete the calculation for these plants.

The parameter TYPE defines a plant type (TYPE=3: annual legume crop, TYPE=4: perennial legume crop). Additional to the organic bound amount of the residues (N_{res}^{org}) as part of the total amount of N in residues (N_{res}^{tot}), CANDY considers a certain amount of inorganic N that is equally deposited in the subsoil:

$$N_{res}^{org} = N_{res}^{tot} \cdot (1 - LNDSUB)$$

LNDSUB part of N deposition in subsoil [0…1]

The fixation of atmospheric nitrogen is given by:

$$N_{sym} = N_{dem} \cdot (1 - LNUTOP)$$

$$N_{soil_up} = N_{dem} - N_{sym}$$

N_{sym}	daily N uptake from symbiotic fixation	[kg N ha^{-1}]
N_{dem}	daily N demand	[kg N ha^{-1}]
N_{soil_up}	daily N uptake from soil N_{min} pool	[kg N ha^{-1}]
LNUTOP	part of N uptake from soil N_{min} pool	[0…1]

Intercropping (zalf_zf)

Requires additional parameter table cdyzfprm (not contained in standard edition)

Symbol	**description**	**unit**
VARIANTE	Sub name	string
K_STR	Controls build up rate depending on global radiation (std value 0.3)	(dtDM ha^{-1})/ (MJ m^{-2})
K_TOT	Controls break down rate depending on temperature (std value 0.5)	K^{-1}
T_MIN	Crop breaks down if air temperature drops below this limit (std value 0)	°C

T_KIL	Crop is finished if air temperature falls below this limit (std value -9)	°C
SNOW_KRIT	Critical level for snow cover to change temperature limit (std value 10)	mm water
T_KIL_SNOW	Crop is finished if air temperature falls below this limit and snow is above the critical level (std value -5)	°C
N_GEHALT_T	N concentration in crop biomass (std value 3.4)	kg N / dtDM

The module implements a new method to calculate N demand together with crop biomass.

$$\Delta BM = R_{growth} - R_{breakdown}$$

$$R_{growth} = K_{str} \cdot GLOB$$

$$R_{breakdown} = \begin{cases} K_{tot} \cdot (T_{min} - T) & T < T_{min} \\ 0 & T \geq T_{min} \end{cases}$$

$$N_{dem} = \Delta BM \cdot N_{BM}$$

CANDY_T approach for transpiration-controlled growth

The module implements a simple method to calculate N demand as proportional to transpiration. As ancestor, it provides this method also to *cdydgrn* which is then completed with some additional procedures.

Permanent Grassland (cdydgrn)

Input

symbol	**description**	**unit**	**source**
LTEM	daily air temperature	[°C]	cdy_cldat
TRa	actual transpiration	[mm]	internal
iLCU	increase of livestock units	number	cdymadat (macode=10)
dLCU	decrease of livestock units	number	cdymadat (macode=11)

Output

symbol	description	unit	measurement id	result id
N in mulch	Amount of N	kg/ha	50	
C in mulch	Amount of C	kg/ha	51	
DM yld	Dry matter yield	dt/ha	26	
N yld	Nitrogen yield	kg/ha	29	
NPP	Net prime production			137

Parameters (see also those in *cdycrops*)

symbol	description	unit	source
TRANSKO	transpiration coefficient	[kg]	cdycrops
TS1	threshold 1 of temperature sum	[°C]	cdycrops
TS2	threshold 2 of temperature sum	[°C]	cdycrops
TK_MIN	minimum of transpiration coefficient	[kg mm^{-1}]	cdycrops
TK_MAX	maximum of transpiration coefficient	[kg mm^{-1}]	internal
C_INP	carbon-FOM input from animal faeces for 1 animal unit	[kg ha^{-1} d^{-1}]	cdylives
FOM_ID	item_ix of FOM from animal faeces	[-]	cdylives
N_UPT	nitrogen uptake from plant biomass for 1 animal unit	[kg ha^{-1} d-1]	cdylives

Description

Permanent grassland starts with sowing and ends with ploughing up. In between the grassland is managed by several cuts over the year with an optional grazing from livestock. In addition, grassland is characterised by long vegetation duration. The main drivers for grassland development are air temperature (ATEM) and actual transpiration:

$$TS_i = TS_{i-1} + ATEM - 4 \quad ; \; ATEM > 4$$

$$TK = \begin{cases} TK_{max} & ; \quad TS \leq TS_1 \\ TK_{min} + (TK_{max} - TK_{min}) \cdot \frac{TS_2 - TS}{TS_2 - TS_1} & ; \quad TS_1 < TS < TS_2 \\ TK_{min} & ; \quad TS \geq TS_2 \end{cases}$$

In permanent grassland CANDY simulates a continuous C flux from roots to soil organic matter. If root mass regenerates twice during vegetation time (VEGDAU), the FOM deposition (C_{fom_root} from grass roots is:

$$C_{fom_root} = 2 \cdot \frac{C_{ts_root} \cdot FIX_R}{VEGDAU}$$

This raises a certain N demand for the below ground part of the crop considering the crop cover degree (CC) and the C/N ratio of root material (CNR_{root}):

$$N_{bg} = CC \cdot \frac{C_{fom_root}}{CNR_{root}}$$

and is raising the provisional daily N demand, that is controlled by the transpiration TR_a:

$$\widehat{N}_{dem} = TK \cdot TR_a + N_{bg}$$

For stability reasons $\widehat{N}_{dem}$ is limited to a daily rate of 4 kg/ha. Moreover, the final N demand is reduced by symbiotic fixation, that leaves the part f_{lf} as potential uptake from soil profile, while the rest should be provided by symbiotic fixation N_{sym} of the legume part in the crop:

$$N_{dem} = \min(4, \widehat{N}_{dem}) \cdot f_{lf}$$

$$N_{sym} = N_{dem} \cdot (1 - f_{lf})$$

The actual daily N-uptake into crop depends on this demand and the supply provided by soil mineral N. The symbiotic fixation is reduced to 10% of its previous value if the supply is 10 kg/ha higher than the actual demand. Further, the actual N uptake from soil will be reduced if the supply is lower than the demand. The finally calculated N uptake N_{upt} may be lower than the expected demand. Therefore, the actual N flux into the background biomass $\widehat{N}_{bg}$ is reduced:

$$\widehat{N}_{bg} = N_{bg} \cdot \frac{N_{upt}}{N_{dem} + N_{sym}}$$

This flux is split between rhizodeposition (N_{fom_root}) and root growth (N_{bm_root}) where root growth is limited to 50% of the rhizodeposition N flux.

Finally, N_{upt} is added the above ground N pool of the grass crop N_{gbm}, considering the N flux for root deposition and root growth:

$$N_{gbm} = N_{gbm} + N_{upt} - N_{fom_root} - N_{bm_root}$$

That is transformed into the amount of aboveground dry matter (DM)

$$DM = \frac{N_{gbm}}{N_GEHALT}$$

TS	temperature sum	[-]
ATEM	daily air temperature	[°C]
TK	daily transpiration coefficient	[kg mm^{-1}]
TS_1	threshold 1 of temperature sum	[°C]
TS_2	threshold 2 of temperature sum	[°C]
TK_{min}	minimum of transpiration coefficient	[kg mm^{-1}]
TK_{max}	maximum of transpiration coefficient	[kg mm^{-1}]
N_{up}	N uptake of plant	[kg ha^{-1}]
TR_a	actual transpiration	[mm]

After a cutting action the crop cover is set to 0.2 and the crop height as well as Ngreen are adapted according to the cutting intensity while root amount is not changed.
Cutting intensity can be given in terms of cutting height (in cm) above ground or as part of aboveground biomass being cut (in%). Cutting height must be given in the value column while the part is taken from the quantity (DB-table column origval). These inputs must be seen as alternatives. It is recommended to set quantity to -1 if cutting height should be considered by the model. As an exception, the model assumes a complete removal of aboveground biomass (part=100%), if both input data (quantity as well as value) are set to zero.
After a cupping cut, the aboveground matter is added to the mulch as green matter. The same happens after freezing.
If scenario simulations are performed without exact knowledge of cutting dates, the crop can set to *autoharvest* mode, changing the parameter *type* from 5 to 6. Now the system calculates a temperature sum that has to reach a trigger level to start a cutting action. The second condition is that the amount of biomass is above a critical level (N_{green} > 25 kg/ha). The default values for the temperature sum values that lead to cutting are:

1	785
2	1360
3	2230
4	2870
5	3460

These trigger levels can be adapted over the management data implementing a (fake) cutting record with a date after sowing and well before the first cutting event is expected where *quantity* contains the temperature sum and *value* the corresponding number of the cutting. Here, *quantity* and *value* refer to the headers in the management tab of the GUI. In the table *cdy_madat* the parameters can be found in the columns *origval* (temperature sum) and *amount* (number of cutting).

The model can apply fertilizer automatically if the autofertilizer option is activated together with autocut. This can be organic amendments, mineral nitrogen or a combination of both. The applied amount is related to the N offtake from the last cut and will be applied at the same day as the cutting event. The model call has to include the parameter *PGLOM*.

PGLOM=0	all N is applied as mineral fertilizer
PGLOM=1	all N is applied as organic amendment (item_ix=1) if N>50kg/ha otherwise, it is added to next application amount.
PGLOM=2	N is applied as organic amendment if N> 50 kgN/ha; otherwise, it is applied in mineral form.
PGLOM=3	all N is applied as organic amendment (item_ix=1) if N>50kg/ha otherwise, it is added to next application amount.; no limitation

for the annual added organic N but each application after cutting is reduced according to the value of dng_eff

In PGLOM 1 and 2 all organic amendments are limited to 170 kg N ha^{-1} yr^{-1} according to the German law. This restriction is not valid for PGLOM=3.
All 'regular' fertilization events in the management data will be executed as usual. The amount of mineral N fertilizer can be modified changing the parameter *dng_eff* in *cdyaparm*.

If the number of animal units is not null, the biomass N pool is reduced due to grazing with the amount of N uptake by animals given in the parameter N_UPT. Animal faeces are treated as organic amendments. The specific addition of organic matter is described by the parameters OD_ID (quality) and C_INP (quantity). Animal units that are defined in the table CDYLIVES can be located and relocated to/from the grassland as a management activity.

$N_{AU} = N_{AU} + \Delta N_{AU}$

$N_{GR} = N_{AU} * N_UPT$

$C_{OA} = N_{AU} * C_INP$

N_{AU}	number of animal units	[-]
N_{GR}	N uptake by grazing animals	[kg ha^{-1}]
C_{OA}	carbon flux to soil with fresh organic matter from animal faeces	[kg ha^{-1} d^{-1}]
N_UPT	specific N uptake (parameter)	[kg ha^{-1} d^{-1}]
C_INP	specific C input from faeces	[kg ha^{-1} d^{-1}]

Permanent Grassland II (cdypgl)

Input

symbol	description	unit	source
ATEM	daily air temperature (T_{air})	[°C]	cdy_cldat
iLCU	increase of livestock units	number	cdymadat (macode=10)
dLCU	decrease of livestock units	number	cdymadat (macode=11)

Output

symbol	description	unit	measurement id	result id
N in mulch	Amount of N	kg/ha	50	
C in mulch	Amount of C	kg/ha	51	
Abg_DM	Above ground DM	dt/ha	59	
DM yld	Dry matter yield	dt/ha	26	
N yld	Nitrogen yield	kg/ha	29	
NPP	Net prime production			137

Parameters (see also those in *cdycrops*)

symbol	description	unit	source
TRANSK	Specific growth rate μ_0	[dt ha^{-1}]	cdycrops
TS1	Minimum DM above ground	[dt ha^{-1}]	cdycrops
TS2	Maximum DM above ground	[dt ha^{-1}]	cdycrops
TK_MIN	air temperature to kill living BM	[°C]	cdycrops
SLOPE	N-stress coefficient (α)	[-]	cdycrops
FIX_R	Max. C-amount in roots	[kg ha^{-1}]	cdycrops
C_INP	carbon-FOM input from animal faeces for 1 animal unit	[kg ha^{-1} d^{-1}]	cdylives
FOM_ID	item_ix of FOM from animal faeces	[-]	cdylives
N_UPT	nitrogen uptake from plant biomass for 1 animal unit	[kg ha^{-1} d-1]	cdylives

Description

cdypgl is very similar to cdydgrn. Mainly, the growth process differs from the previous submodel. Building of biomass is described as a logistic growth process driven by air temperature (T_{air}) where the relative growth rate is modified by the N concentration in the green biomass (N_{conc}) and water stress (AET/PET) .

If $DM<DM_{max}$ and $T_{air}>4$ the daily growth rate is given by

$$dDM = \mu_0 \cdot T_{air} \cdot DM \cdot (1 - \frac{DM}{DM_{max}}) \cdot (1 - \exp(-\alpha \cdot N_{conc})) \cdot \frac{AET}{PET}$$

otherwise dDM=0.

Generic crop growth model (agro1)

Additional parameters

symbol	description	unit
From table ***cdyacrop***		
item_ix	ID	-
alpha	Photosynthetic capacity per unit leaf nitrogen	µmol CO_2 s^{-1} $(gN)^{-1}$
beta	Photosynthetic rate at light saturation	µmol CO_2 m^{-2} s^{-1}
sigma	Controls LAI development in the second development phase (maturing, DVI>1)	-
t_upl	Upper temperature limit for photosynthesis	°C
t_lol	Lower temperature limit for development	°C
t_opt	Optimum temperature for photosynthesis	°C
n_seed	Initial N at sowing	kg/ha
c_seed	Initial C at sowing	kg/ha
ncr_bm	N:C ratio in green biomass	-
ref_ts	Accumulated temperature above the lower limit	°C
ts_emg	Temperature sum at emergence	°C
senescence	Partial LAI breakdown	-
sp_lf_ar	Specific leaf area	m^2kg^{-1}
cov2lai	Conversion factor crop cover : LAI	-
gr_resp	Growth respiration	g g^{-1}
spch	Specific crop height	$kgha^{-1}m^{-1}$
sprd	Specific root depth	$kgha^{-1}m^{-1}$
m	Determines the shape of temperature response curve for photosynthesis	-
b	C3 crop: 0.8 C4 crop: 0.4	-
From table ***cdyacrdp***		
kex	Extinction coefficient (DVI dependent)	-
prt	Partitioning factor main prod.(DVI dependent)	-
prx	Partitioning factor root (DVI dependent)	-
plx	Partitioning factor leaf (DVI dependent)	-
bbch	development state in BBCH code (DVI dependent)	-
ndfa	Partitioning factor for legume N fixation (DVI dependent)	-

The formulation of this module is mostly based on the description of the model AGRO-C by Yao Huang et al. DOI: 10.1016/j.agrformet.2008.07.013 where most formulas are taken from and repeated here to provide better understanding.
In principle, the model must describe the same blocks that are shown in Figure 15 plus the calculation of development state.
Crop development is quantified by the development index (DVI) calculated from the daily mean air temperature *T* and an accumulated reference temperature *ref_ts*

$$DVI = \sum \frac{T}{abs(ref_ts)} \; ; \; if \; T > T_{lol}$$

With a negative value for *ref_ts* in the parameter table the model activates the *autoharvest* option. That means the harvest action will be triggered at DVI=2 when the development is completed. Still, a harvest event in the management data has higher priority. This way, harvest can be executed before a full completement of development. Any later harvest event will be ignored because there is no longer a crop in the system.
There is no information from management data about the processing of potential by-products, if *autoharvest* is executed. The standard rule is that only stubble are left on the field and all other biomass is removed. An extension of the model's name in table *cdycrops* can solve this problem. The last character in the extended model's name can be set to 1 or 0. The value '1' signals that the by-product is used while the value '0' signals that all crop residues are left on the field. To separate this switch from the model's name itself we recommend a construction like agro1#1 or agro1#0.

Crop growth is based on photosynthesis quantified by photosynthetic photon flux density *PPFD [µmol m^{-2} s^{-1}]*

$$PPFD = 2.3 \cdot 10^6 \cdot \frac{GLOB}{24 \cdot 60 \cdot 60}$$

The intercepted radiation depends on leaf area index LAI, the canopy reflectance *refl* (assumed to be 0.6) and the crop specific and development dependent irradiance extinction coefficient k_{ex} :

$$PARX = (1 - refl) \cdot PPFD \cdot \frac{1 - exp(-k_{ex} \cdot LAI)}{k_{ex} \cdot LAI}$$

The daily photosynthesis rate DPR depends on PARX and is further moderated depending on temperature stress (rf_T), water stress (rf_W), atmospheric CO_2 concentration (rf_C) and nitrogen state of the crop (N_{leaf}) as given by Huang et al. (2009)

$$DPR = \frac{\alpha \cdot N_{leaf} \cdot rf_T \cdot rf_W \cdot rf_C \cdot PARX}{\beta + PARX}$$

Atmospheric CO_2 concentration is taken from the table cdy_clcng (see database manual).

Mean values of temperature at night (T_n) and during daylight (T_d) must be estimated, if climate data contain only the average temperature:

$$T_n = -0.4 + 0.98 \cdot T$$
$$T_d = \; 0.9 + 1.05 \cdot T$$

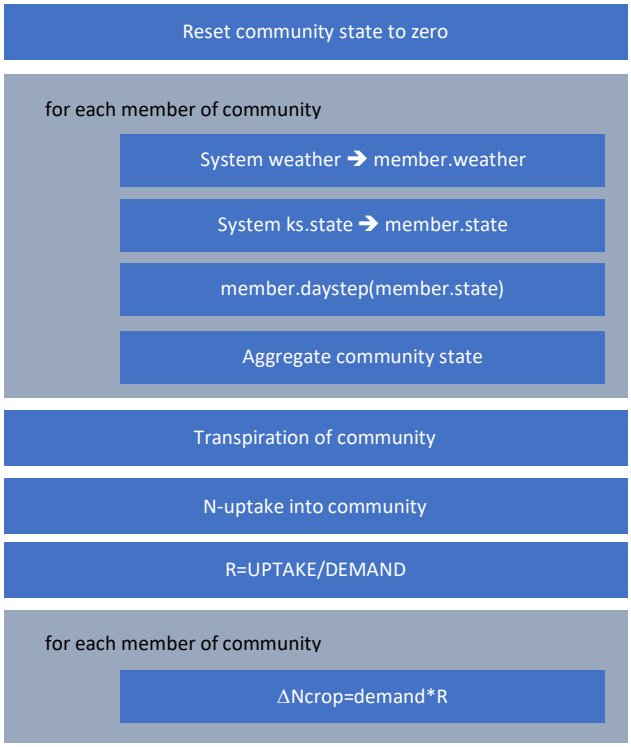
The temperature dependence of photosynthesis is taken from Straskraba/Gnauk: *Aquatische Ökosysteme* p.118:

$$rf(T) = \left(\frac{T_{max}-T}{T_{max}-T_{opt}}\right)^{x} exp\left(x \cdot \left(1 - \frac{T_{max}-T}{T_{max}-T_{opt}}\right)\right)$$, where x=10*m; T_{max}≈47 ; T_{opt}≈36 ; T=T_d

The effect of soil water supply on reduction of photosynthesis is slightly adapted from the description given by Huang et al., 2008 .
The coefficient $rf_w$is applied to express the reduction of daily photosynthesis rate due to a reduced soil water amount using the sums of relevant variables over the rooted soil layers.

$$rf_w = min\left(1, max\left(0.1, \frac{\sum_i \theta_i - \sum_i PWP_i}{\sum_i FC_i - \sum_i PWP_i}\right)\right)$$

The subtraction of respiration (growth and maintenance) from the gross primary production GPP leaves the daily net prime production NPP that is accumulated and gives the base for further calculations of crop state variables.
DVI dependent partitioning coefficients describe how the daily NPP is distributed between roots, leaves, main product and -in case of legumes- N-fixing rhizobium. Crop height and rooting depth will then be determined according to the specific crop height or root depth that are given in the parameters.
Furthermore, the daily NPP controls the N demand of the growing crop using the N to C relation of parameter for the biomass.
For legume crops, a DVI-depending part of the daily NPP will be used to feed the symbiotic bacteria. It is assumed that 7 kg C are required to deliver 1 kg N to the crop.



Intercropping (crop communities)

Figure 18 : schematic representation of the daystep routine for a crop community

Intercropping is implemented based on the agro1 model approach. Additional actions are required to build up a community of several crops:
Sowing intercrop member (action_id=21) adds a specific crop (of agro1 type) as given part (in %) of a crop community. Each member can be individually harvested with residues removed (action_id=22) or left on field (action_id=29).
The model builds a list of intercrop members that is handled like a 'normal' crop using aggregated values for the crop properties: maximum for rooting depth and crop height and sum for interception capacity and crop coverage, considering the part of each member. Within the global daystep routine (see Figure 18) is simulated the specific daystep for each member of the crop community one after another aggregating the resulting nitrogen demand. If enough nitrogen is not available, the individual demand of each member is reduced according to the relation between total demand and soil supply.

Obviously, all CANDY routines for data output (beside harvest results) with observations and results relate to the community as a whole because the data structure allows not to focus on a single member of the community.

Soil structure dynamics

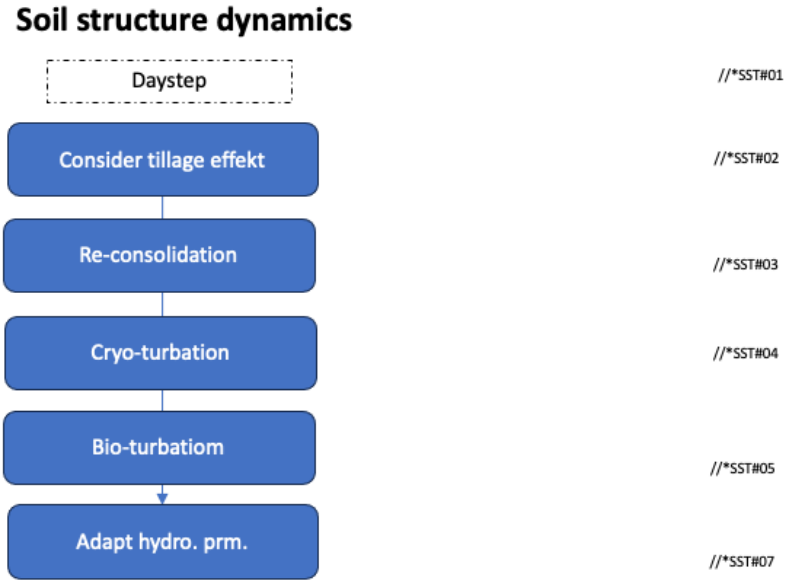


Figure 19: daystep in soil structure module

Input

symbol	description	unit	source
P	daily precipitation	[mm]	CDY_CLDAT
T_{air}	daily mean air temperature	[°C]	CDY_CLDAT
BAT	Biologic Active Time	[d]	internal

Output

symbol	description	unit	measurement id	result id
BD	bulk density	[g cm^{-3}]	63	704 (0-3 dm)
PD	particle density	[g cm^{-3}]	64	
PV	pore volume	[Vol. %]	65	
FC	field capacity	[Vol. %]	61	
PWP	permanent wilting point	[Vol. %]	62	

Parameters

symbol	description	unit	source
f_bioturb	optional parameter to convert BAT into daily bulk density change	g cm^{-3} d^{-1}]	CDYSSDPA

Some other parameters are determined internally.

Description

Further enhancement of the CANDY model system is related to the implementation of a module for the dynamic description of soil structure.

Please be aware that this module is still under development and may require special calibrations to different site conditions.

If this option is activated, the following parameters of soil structure become state variables:

- Bulk density (BD)
- Particle density (PD)
- Pore volume (PV, defined by BD and PD)
- Field capacity (FC)
- Permanent wilting point (PWP)

The soil parameters must be quantified with an additional specification of the C_{org} content that relates to these values and the site-specific value of aggregate density as a maximum value for soil compaction.

Field capacity and permanent wilting point are calculated using the van Genuchten approach for the water retention curve with the pedotransfer function (PTF) that is specified in the ini file. The residual water content is adapted to stone content according to approaches by Wösten et al. (1999) and Chirico et al. (2007). Further description of the implemented functions is given in chapter *Pedotransferfunctions in CANDY*.

Bulk density as co-driver for soil structure

Soil structure depends on bulk density (BD) and the organic carbon concentration of soil. The BD is influenced by management activities and climatic conditions. Soil loosening (disaggregation) occurs because of soil tillage, bio- and cryoturbation. Further technical compaction is neglected at this model stage. A re-compaction takes place because of natural processes, such as sedimentation of soil, and technically caused by the load of agricultural machineries.

Soil loosening by tillage and the natural re-compaction are described with model approaches of Schaaf (1998).

Soil loosening

$$\rho_b = \hat{\rho}_b - ef \cdot (\hat{\rho}_b - \frac{2}{3}\rho_0)$$

$\rho_b, \hat{\rho}_b$	bulk density [g cm^{-3}]	
ρ_0	bulk density after complete re-compaction	[g cm^{-3}]
ef	loosening efficiency of soil tillage tool	[0..1]

Re-compaction

$$\rho_b = \hat{\rho}_b + \cdot (\rho_0 - \hat{\rho}_b) \cdot \left(\frac{R}{R + exp(3.735 - 0.08835 \cdot h)}\right)$$

$\rho_b, \hat{\rho}_b$	bulk density [g cm^{-3}]	
ρ_0	bulk density after complete re-compaction	[g cm^{-3}]
R	factor of re-compaction	*[-]*
h	*lower boundary layer*	*[dm]*

The factor of re-compaction (R) results from water percolation, depth and sand content of the corresponding horizon and provides the possibility to calculate the actual bulk density:

$$R = P \cdot \left(\frac{1 + 2\frac{S}{S + \exp(8.587 - 0.075 \cdot S)}}{(10 \cdot h)^{0.6}}\right)$$

R	factor of re-compaction	[-]
P	water percolation	[mm]
S	sand content	[%]
h	layer height [dm]	

The bulk density after re-compaction (BD_0) is calculated by an approach of Ruehlmann and Körschens (2009) depending on actual C_{org} content at every time step:

$$BD = (2.631 + 15.811 \cdot b) \cdot \exp(b \cdot C_{org})$$

The parameter b is determined site specifically during model initialisation. Usually, the observed BD is related to a specific sedimentation status of the soil.
Consequently, it is necessary to implement a re-compaction level:

$$BD_0 = BD(C_{org}) \cdot RC$$

BD_0	bulk density after complete re-compaction	[g cm^{-3}]
RC	re-compaction level	[> 0]
$BD(C_{org})$	observed tuple BD , C_{org}	[g cm^{-3}]

For practical reasons, bulk density measurements are usually not performed on a recently loosened soil. Therefore, RC will be close to 1.

Cryoturbation

If the frozen soil water is thawing within one time step, the volume change is included into the bulk density calculation:

$$PV = \varepsilon_L + \varepsilon_W \cdot 1.09$$

$$\rho = (1 - PV) \cdot PD$$

PV	pore volume after thawing	[0…1]
ρ	soil bulk density	[g cm^{-3}]
ε_W	relative water volume	[0…1]
ε_L	relative air volume	[0…1]
PD	particle density	[g cm^{-3}]

Bioturbation

The results of bioturbation are calculated assuming that the change of bulk density is related to the actual BAT value:

$$\Delta BD = f_bioturb \cdot BAT$$

ΔBD	change of bulk density (old-new)	[g cm^{-3}]
f_bioturb	parameter	[g cm^{-3} d^{-1}]
BAT	Biologic Active Time	[d]

The parameter *f_bioturb* can be defined in the parameters for soil structure dynamics (CDYSSDPA) – otherwise the standard value 0.001 is used.

Adaptation of hydrologic parameters

The pedotransfer functions as described later in this document (see p. 75 ff) are used with the texture parameters and current values of SOC and BD to daily update particle density (PD), pore volume (PV, defined by BD and PD), field capacity (FC), and permanent wilting point (PWP) in each top soil layer. The transformation from hydrologic potential h to volumetric soil moisture values of PWP and FC is performed using the van Genuchten approach: $\theta(\psi) = \theta_r + \frac{\theta_s - \theta_r}{(1+(\alpha \cdot |\psi|)^n)^m}$ for matric potential ψ of $10^{4.2}$ and $10^{1.8}$,respectively, together with θ_r, θ_s, n, m, and α from the selected hydrologic pedotransfer function.

Mulch layer

The mulch layer behaves like a storage facility where organic matter is collected and step by step transferred to the first soil layer. The input consists of stubble that are left after harvest and dead plant material that was killed by freezing (intercrop,

grassland). There is no matter turnover simulated and therefore all matter keeps its original properties. The material is completely transferred to soil with a tillage action or in small parts during the *daystep* routine. This flux implemented as an organic amendment where the C amount is calculated depending on air temperature:

$$\Delta C_i = \begin{cases} C_i \cdot k_{mulch} \cdot 2.1^{\frac{T-35}{10}} & T > 0 \\ 0 & T \leq 0 \end{cases}$$

With
$C_{i.}$: carbon amount of a mulch pool
T : air temperature
k_{mulch} : transfer coefficient

Soil organic matter turnover

Soil organic matter turnover is considered as a main driver of soil functions considering the close link to soil structure and nitrogen transformation.
In general, we differentiate the fresh organic matter (FOM) that comes from external sources in a widely spread variation of properties and the soil organic matter (SOM) that is usually in focus if we talk about carbon storage in soils but strongly related to the soil biology. The microbial driven turnover is determined by the carbon flux where nitrogen fluxes are controlled by the C/N ratio.
Beside other properties each FOM is characterized by parameter describing its potential to reproduce SOM. This input is here called the C_{rep}-flux that can beaded for the different sources. Obviously, a higher C_{rep}-flux is required to increase carbon storage. Beside this, the final amount of SOM is controlled by environmental conditions. It is a special feature of the CANDY model to quantify the environmental conditions as Biological Active Time (BAT) and this way provide a mean to characterize a given site.
Altogether, the results about SOM, C_{rep} and BAT provide means to assess the soil carbon storage function for a special management / site combination.

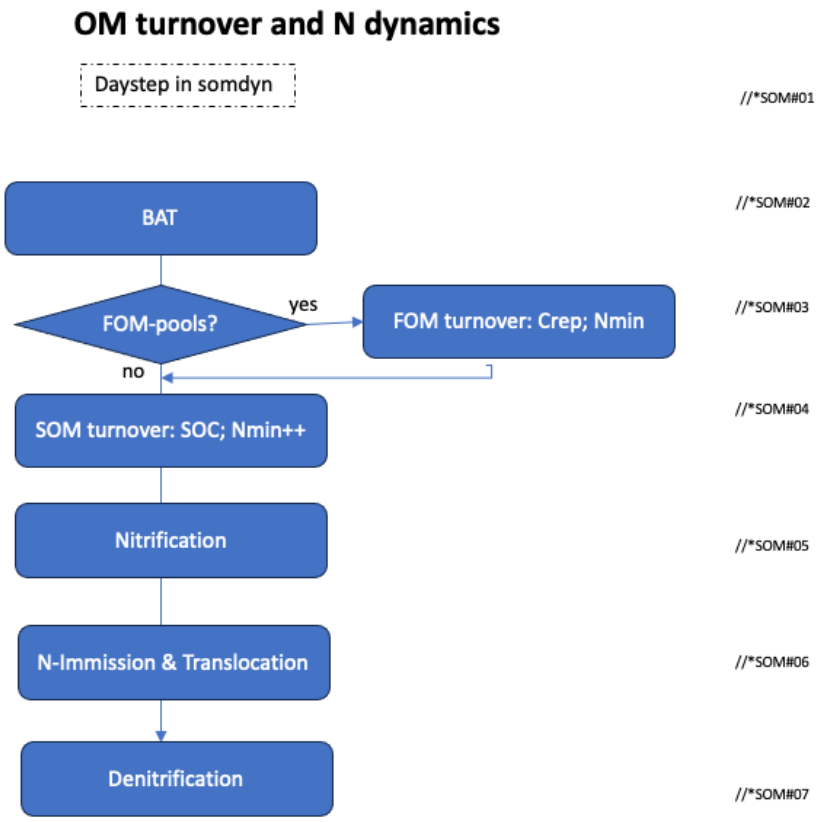


Figure 20: daystep for OM turnover and coupled N-Dynamics

Biologic Active Time

Input

symbol	description	unit	source
T	soil temperature	[°C]	Internal
ϴ	soil moisture	[Vol. %]	Internal
FPART	clay and fine silt (particles ≤ 6.3 µm)	[M. %]	cdy_hrzn
h	depth of the calculation layer in soil	[cm]	Internal

Output

symbol	description	unit	measurement id	result id
BAT	Biologic active time	[d]	52	104

Description

Biologic active time (BAT) is a concept that describes the impact of environmental conditions on biologic activity on soil organic matter (SOM) turnover (Franko et al. 1995). In each time interval, a certain biologic activity in a suboptimal environment will produce a specific turnover result lower than under optimal conditions. The same

results occur when the time interval is split in BAT and non-BAT. During the BAT interval the microbial activity is only limited by the substrate, while during non-BAT there is no activity at all. For the calculation of the BAT interval, the effects of soil temperature, soil water and soil aeration are considered. The annual BAT sum is an important indicator for the potential turnover under the given conditions.

The scheme in Figure 21 demonstrates the principle how different intensities of uniform time steps (Figure 21A) are transformed into time steps of different length and uniform intensity (Figure 21 B). The calculated turnover, symbolised by the bar area, will be the same for both approaches, anyway. In the latter case (B) the new calculated time step (Δt') is a product of the reduction function R(t) and the origin time step (Δt). In this case the non-BAT time step is represented as the blank space between the BAT bars (Figure 21 B).

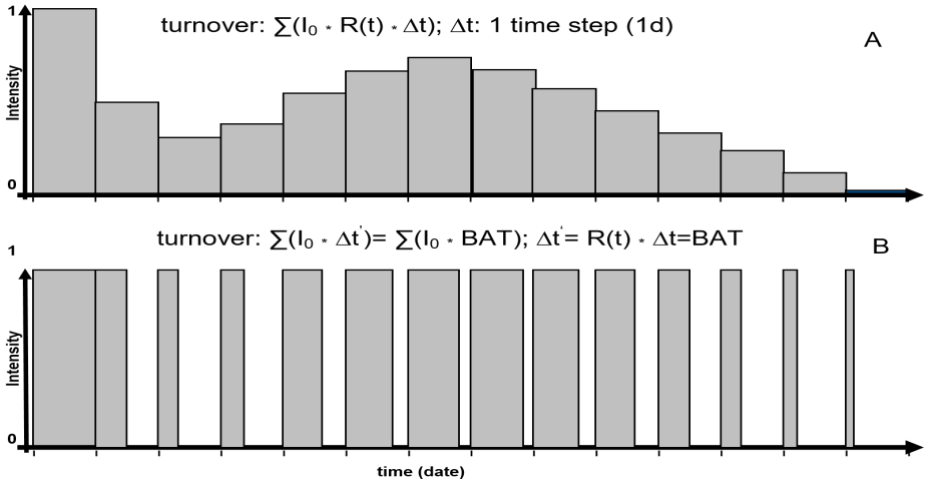


Figure 21: Schematic representation of the turnover calculation by the standard approach (A) and the BAT approach due to transformation of time steps (B).

Total BAT is calculated in daily time steps for the topsoil (usually 0-30 cm) as the sum of BAT in single layers BAT_i considering the impacts of temperature $f(T_i)$ water $f(W_i)$ and aeration $f(A_i)$.

$$BAT_i = f(T_i) \cdot f(W_i) \cdot exp(-f(A_i) \cdot d) \quad \text{with } d = \begin{cases} 0.5 \cdot h & i = 1 \\ h & i > 1 \end{cases}$$

The impact of soil temperature varies from 0 to 1 and includes the following thresholds (in centigrade):

$$f(T) = \begin{cases} 0 & ; \quad T < -20 \\ 2.1^{\wedge}\left(\frac{T-35}{10}\right) & ; \quad -20 < T < 35 \\ 1 & ; \quad T \geq 35 \end{cases}$$

The impact of soil water in layer *i* depends on the relative filling (p) of the pore volume (PV) with water (W)

$$p_i = \frac{W_i}{PV_i}$$

$$f(W_i) = \begin{cases} 4 \cdot p_i \cdot (1 - p_i) & if \quad p_i < 0.5 \\ 1 & if \quad p_i \geq 0.5 \end{cases}$$

A further impact of water is lack of aeration f(A) that depends on the air volume (V_a), the pocket volume (V_{pk}), the height of a calculation layer (h = 10 cm) and a proxy (c) for the effect of reduced oxygen in the layer above the upper boundary condition.

$$f(A_i) = f(A_{i-1}) + \sqrt{\frac{f(D_i) \cdot f(T_i) \cdot f(W_i)}{h \cdot V_{ai} \cdot c_i \cdot (V_{ai} - V_{pk})}}$$

with:

i=1..smax; $c_i = c_{i-1} \cdot exp(-f(A_{i-1}) \cdot h)$; c_0=1; c_1=1; $f(A_0)$=0;

and the damping factor $f(D_i) = \max(6, \cdot FP_i) \cdot 0.2844 - 1.4586$ that depends on the quantity of fine particles (FP) i.e. clay and fine silt (particles ≤ 6.3 µm) .

If soil is very moist and air volume is lower than pocket volume $f(A_i)$ is set to 100 and c_i to 0.

The pocket volume can be set in the general parameters (*cdyaparm*). If there is specified a negative value (as recommended), V_{pk} is calculated depending on soil properties:

$V_{pk} = PV - 0.98 * \theta_s$

Where

PV: pore volume

θ_s : sat. water content according to the Approach of Rawls and Brakensiek

SOM pool turnover

Input

symbol	description	unit	source
BAT	Biologic Active Time	[d]	Internal
FOM_{inp}	event based C input with FOM	[kg ha^{-1}]	internal

Output

symbol	description	unit	M_IX	RES_IX
C-AOS	Active SOM pool; behaves like microbial biomass	[kg ha^{-1}]		90
C-SOS	Stabilised SOM pool	[kg ha^{-1}]		91
C-LTS	Long term stabilised OM pool; relates to soil structure	[kg ha^{-1}]		95

C_{org}	Soil organic carbon as sum of the three pool	[M. %]	7

Parameters

symbol	description	unit	source
η	synthesis coefficient for a FOM pool	[-]	cdyopspa
k_{FOM}	rate coefficient for a pool of FOM	[d^{-1}]	cdyaparm
k_A	rate coefficient for the C-flux from S-SOM to the A-SOM	[d^{-1}]	cdyaparm
k_S	rate coefficient for the C-flux from A-SOM to S-SOM	[d^{-1}]	cdyaparm
k_m	rate coefficient for the C-mineralisation from A-SOM	[d^{-1}]	cdyaparm
k_d	coeff	[]	cdy_hrzn
λ_{LTS}	coeff	[]	cdy_hrzn

Description

Soil organic matter (SOM) dynamics may be handled by different approaches. The CANDY approach uses conceptual pools and describes C and N dynamics as well.

The SOM pools in the classical CANDY model have conceptual character and are not measurable (Figure 22). Soil organic matter is subdivided into four compartments: (1) fresh organic matter (FOM), (2) biological active soil organic matter (A-SOM or AOM), (3) stabilised soil organic matter (S-SOM or SSM) and (4) long term stabilised soil organic matter (LTS-SOM). After each time step the resulting pool size for C_{org} can be recalculated from the sum of all SOM pools. All processes of the C turnover are formulated as first-order reactions (Franko et al. 1995). The model may handle up to six different FOM pools. A part of FOM is transferred into SOM. The relation of the SOM production to the FOM decay is described by the synthesis coefficient (η). The flux from FOM into A-SOM is called C_{rep}. The A-SOM pool decays with a rate coefficient (k_{AOM}). In addition to this, C loss to carbon dioxide, another flux from A-SOM to S-SOM, is modelled with the coefficient k_{SOM}.

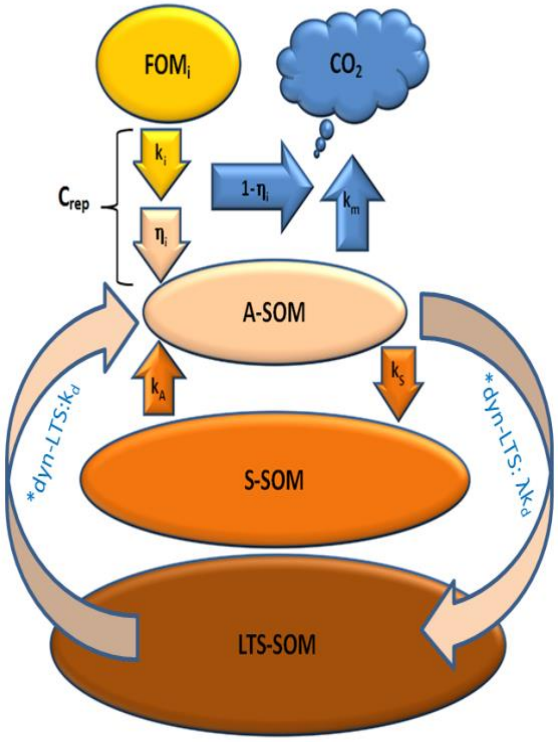


*Figure 22: Conceptual pools and fluxes within the soil organic matter module in CANDY ; *dyn-LTS: description see text.*

All processes of the C turnover are formulated as first-order reactions (Franko et al. 1995). The decomposition of fresh organic matter is determined by its turnover coefficient k_{FOM}:

$$\frac{dC_{FOM}(t)}{dt} = \dot{C}_{FOM} = k_{FOM} \cdot C_{FOM}(t)$$

The FOM decomposition results in the creation of A-SOM. The carbon flux from FOM into A-SOM is called C_{rep}. The relation between A-SOM production and FOM decay is described by the synthesis coefficient η_{FOM}:

$$\frac{dC_{rep}(t)}{dt} = \dot{C}_{rep} = \dot{C}_{FOM} \cdot \eta_{FOM}$$

The turnover of the active SOM pool includes the reproduction flux from FOM (C_{rep}), the mineralisation to CO_2 (coefficient k_m) and an internal matter exchange with the stabile SOM pool (turnover coefficients k_a and k_s), using the general parameters k_m=0.00556 d^{-1}, k_a=0.00032 d^{-1}, and k_s=0.0009 d^{-1}:

$$\frac{dC_A(t)}{dt} = \dot{C}_A = \dot{C}_{rep} + k_a \cdot C_S(t) - k_s \cdot C_A(t) - k_m \cdot C_A(t) - \dot{C}_{LTS}$$

Consequently, the carbon turnover of the stable SOM pool is:

$$\frac{dC_S(t)}{dt} = \dot{C}_S = k_s \cdot C_A(t) - k_a \cdot C_S(t)$$

So far, we have described the biologic driven turnover of the A-SOM and S-SOM pool that both are considered the easy decomposable part of SOM. The SOM that is left has a very low turnover rate that is not so much controlled by biochemical recalcitrance but a result from physical protection in the micro pores of the soil where microbial activity is strongly limited. Following the rationale of the CIPS Model (Kuka et al.2007, Puhlmann et al. 2006) we assume that SOC is distributed over the inner soil surface and quantify the physically protected part in the micro pores from the relation between micro pore related surface to the total inner surface of the soil. After an attempt to describe the LTS dynamics only with the change of the micro pore space as driven by changing SOC concentration, explained by Franko and Merbach (2017), we assume a dynamic soil structure where the relation between micro pores and total soil porosity may be constant but with an exchange of the surfaces in the different pore size classes. The underlying process is comparable to the formation and destruction of soil aggregates where inner aggregate matter is transferred to intra aggregate positions and vice versa. This process is not directly related to the microbial turnover and therefore not depending on BAT. We assume that a part of the new formed SOM is captured inside the micro pores while another part is released from the protection/occlusion to take part in the microbial turnover.

Furthermore, a matter flux through the LTS pool is considered. Assuming the LTS-SOM dynamic is controlled by soil physics, the pool size calculation is ruled by following equations:

$C_{LTS} = C_{MIP}$
with:

$$C_{MIP} = C_{org} \frac{A_{micro}}{A_{micro} + A_{meso} + A_{macro}}$$

$$A_m = 2 \cdot \frac{V_m}{R_m} \quad m \in \{micro, meso, macro\}$$

C_{LTS}	carbon content of corresponding compartments of SOM	[kg C ha^{-1}]
FAT	clay and fine silt (particles < 6.3 µm)	[M. %]
C_{MIP}	carbon amount allocated in micropores	[M. %]
A_m	pore surface area of micro, meso and macropores, respectively	[m^2]
V_m	volume of specific pore space class (micro: PWP, meso: FC-PWP, macro: PV-FC)	[m^3]
R_m	equivalent pore radius ($5 \cdot 10^{-7}$, $10 \cdot 10^{-7}$ and $500 \cdot 10^{-7}$ for micro, meso and macropores, respectively)	[m]

Further details about LTS pool size calculations were given by Kuka et al. (2007), Puhlmann et al. (2006) and Franko et al. (2011).

In the past, the LTS pool was considered to be long-term stable or even inert, assuming that its size remained constant, because changes in its size were expected to be insignificant. Following the ideas of the CIPS model (Kuka et al., 2007) the carbon flux into the micro pore space is restricted to dissolved organic carbon (DOC). Any DOC flux is closely related to microbial activity. The A-SOM pool of the CNP model behaves very similar to soil microbial biomass. Therefore, we assume that the flux between time step t_i and t_{i+1} to/from the LTS pool is affecting the A-SOM pool and hypothesise that:

$$\Delta C_{LTS} = -\Delta C_A = C_{LTS}(t_{i+1}) - C_{LTS}(t_i)$$

Both pools LTS-SOM and A-SOM have a different C/N ratio (γ) meaning that also a flux (N_{flx}) between the mineral nitrogen and an organic N pool must be considered:

$$N_{flx} = \Delta C_A \cdot \frac{\gamma_A - \gamma_{LTS}}{\gamma_A \cdot \gamma_{LTS}}$$

A growing LTS-SOM pool (N-poor) will withdraw C from the N-rich A-SOM pool and set mineral nitrogen free (meaning prevent the mineral nitrogen from being immobilised during the decomposition of fresh organic matter). A decreasing LTS-SOM pool leads to nitrogen immobilisation due to the A-SOM growth and must be considered as N-sink.

Supply of fresh organic matter

The supply of fresh organic matter to the soil results from:

- organic amendments (OA)
- by-products that are left on the field after harvest such as straw and leafs (BP)
- crop residues such as roots and stubble (RT and ST)
- ploughing up of intercrop

The matter flux calculation is based on carbon content in dry matter. All Inputs are first transformed into dry matter and then to C or N (via C/N ratio).

The amount of fresh organic matter input from organic amendments (OA_{fm}) given in the scenario data is multiplied with the according dry matter content.
$OA_{dm} = OA_{fm} * DM_{oa}$

For the other both pathways, we start with basic definitions to calculate the mass fluxes that will be expressed in kg/ha from the given yield data that is given in dt/ha:
$MP_{dm} = Y_{mp} * dm_{mp}$
where
MP_{dm} : dry matter yield of the main product (dt/ha)
Y_{mp} : yield of main product with defined dry matter content (dt/ha)

dm_{mp} : defined dry matter part of the main product [0..1]

The amount of root mass is defined by a linear equation:

$RT_{dm} = FIX_r + BIX * MP_{dm}$

where

FIX_r: yield-independent part of root dry matter (kg/ha)

BIX: Belowground index. Yield-dependent part of root dry matter (kg/dt)

Similar to root dry matter, we assume also for the dry mass of stubble a linear relation to dry matter yield. We have a constant part of stubble dry matter (FIX_s), a yield dependent factor for the total above ground residue dry mass (RIX) and a factor for the stubble part (STIX). The dry matter of by-products is however completely yield dependent:

$ST_{dm} = FIX_s + RIX * STIX * MP_{dm}$

$BP_{dm} = RIX * (1 - STIX) * MP_{dm}$

Where

ST_{dm} : dry matter of stubble (dt/ha)

BP_{dm} : dry matter of by-product (dt/ha)

RIX represents the relation between the yield dependent part of aboveground residues to the dry matter yield of the main product and STIX represents the yield dependent part of stubble in relation to the yield dependent part of all aboveground residues.

For each organic matter input XX (where XX may be OA, BP, ST or RT) the actual element fluxes for C follows from the product of the dry matter amount with the dry matter C concentration of this compartment (C_{dm})

$C_{om} = XX_{dm} \cdot C_{dm}$

Example:

Winter wheat yield=80 dt/ha (reference DM=86%); where straw is left on the field and an amount of 200 dt/ha slurry (pig) is added

Required properties: look up winter wheat in CDYCROPS:

item_ix=9; rt_ix=3009; sh_ix=1009, (the latter both link to cdyopspa.item_ix)

for crop item 9 we find in CDYCROPS:

fix_r=1160 ; bix=16 ; fix_s = 0; rix=93.8; stix=0.1;

for root item 3009 we find in cdyopspa:

c_dm= 0.355

for residue (and stubble) item 1009 we find also in cdyopspa:

c_dm=0.458

the organic amendment with slurry requires the look up of item 156 (slurry (pig)) in **cdyopspa**: *item_ix* to find : dm=0.05 ; c_dm=0.41

Calculation

200 dt/ha slurry as organic amendment

C_{oa} = 200 dt/ha * 0.05 * 0.41 * 100 = 410 kg/ha (*100 to get kg/ha)

By-product: as organic amendment:

(only when action in management is '*harvest, crop res. ploughed*' ! otherwise MP_{dm}=0)

MP_{dm} = 80 dt/ha * 0.86 = 68.8 dt/ha

Straw:

BP_{dm} = 68.8 dt/ha * 93.8 kg/dt * (1 – 0.1) ≈ 5808.1 kg/ha;

C_{bp} = 5808 kg/ha * 0.458 ≈ 2660 kg/ha

Stubbles:

ST_{dm}= 0 kg/ha + 93.8 kg/dt * 68.8 dt/ha * 0.1≈ 645.3kg/ha

C_{st} = 645.3 kg/ha * 0.458 ≈ 295.6 kg/ha

Roots:

RT_{dm}= 1160 kg/ha + 16 kg/dt * 68.8 dt/ha = 2260.8 kg/ha

C_{rt} = 2260.8 kg/ha * 0.355 ≈ 802.6 kg/ha

CANDY calculates the C flux in kg/ha based on mp_dmyield in dt/ha in following statements. Therefore fix_r and fix_s have to be given in kg/ha while bix and rix have the dimension of kg/dt and the C-contents of root and shoot is given as number (value<1).

```
root_c     := ( fix_r+bix*mp_dmyld )*cdm_rt;
byprod_c   := ( rix*(1-stix)*mp_dmyld )*cdm_st;
stubble_c  := ( fix_s+rix*stix*mp_dmyld) *cdm_st;
```

N dynamics

Input

symbol	description	unit	source
N emission	annual N deposition from atmosphere	[kg ha^{-1}]	CDY_FXDAT
N from fertiliser	from mineral fertiliser	[kg ha^{-1}]	CDY_MADAT

Output

symbol	description	unit	mmt_id	result_id
N leaching	downward N loss via percolation through the lower boundary	[kg ha^{-1}]		102
gaseous N loss	total gaseous N loss	[kg ha^{-1}]	-	106
N mineralisation	N_{min} transfer from/to SOM (mineralisation: "+", immobilisation: "-")	[kg ha^{-1}]	-	107
NH_4-N	ammonium nitrogen in specific soil layer	[kg ha^{-1}]	3	-
NO_3-N	nitrate nitrogen in specific soil layer	[kg ha^{-1}]	1	-
NH_4 loss gaseous	ammonia volatilisation	[kg ha^{-1}]	-	123
N_2O emission	N_2O-N emission	[kg ha^{-1}]	75	997

Parameters

symbol	description	unit	source table
N_IM_BEW	immission for cropped land	[-]	CNDAPARM
N_IM_SOM	immission for summer season	[-]	CNDAPARM
SBA parameter set	decision support system for nitrogen fertilisation (ger.: Stickstoffbedarfs-Analyse)	[-]	
CNR_{mic}	C/N ratio of microbial biomass (standard: 8.5)	[-]	CNDAPARM

Description

CANDY considers organic and mineral nitrogen forms. Mineral nitrogen appears as nitrate (NO_3-N) or ammonium (NH_4-N). All organic pools and fluxes are characterized by their C amount and their C/N ratio. The nitrogen fluxes in CANDY result from different source/sink processes (Figure 23).

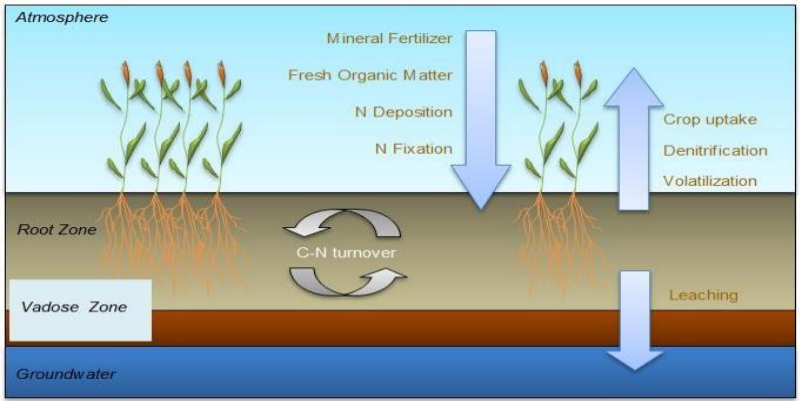


Figure 23: Schematic representation of N dynamics in the CANDY model

The focus of CANDY is on SOM turnover. Nitrogen dynamics are closely related to carbon turnover. However, the characterisation of an agro ecosystem requires a more comprehensive description of sources and sinks:

<u>Sources</u>

➔N deposition from atmosphere
➔Input from land management
- Mineral fertiliser
  - Application of fertiliser
  - auto-fertilisation (goal oriented or SBA method)
- Fresh organic matter
  - organic amendments
  - crop residues

➔C-N turnover
- N-mineralisation(ammonium)
- nitrification

➔crop growth
- N fixation by legumes

<u>Sinks</u>

➔plant uptake
➔N immobilisation in SOM
➔N exports to environment
- N leaching
- gaseous losses (denitrification, volatilisation)

Nitrogen Sources

N deposition

N deposition has to be defined with the basic data as mean annual value. This value will be modified internally according to the actual season (summer: 120 < Julian day < 304) and the vegetation cover (yes/no) in case that the following parameter values have been defined in the CNDAPARM table:

N_IM_BEW (immission for cropped land) ❼ standard: 0.17

N_IM_SOM (immission for summer season) ❼ standard: 0.71

Bare soil: $d\widehat{N}_{im} = \frac{IMMI}{365.25}(1 - N_IM_BEW)$

Covered soil: $d\widehat{N}_{im} = \frac{IMMI}{365.25}(1 + N_IM_BEW)$

$$dN_{im} = \begin{cases} d\widehat{N}_{im} \cdot 2 \cdot N_IM_SOM & 120 < jday < 304 \\ d\widehat{N}_{im} \cdot 2 \cdot (1 - N_{IM_{SOM}}) & otherwise \end{cases}$$

In the case that the parameters are not defined (Null or 0) an equal distribution of N immission over the whole year will be assumed.

Input from land management

Application of fertilizer

The management data (CDY_MADAT) contain the amount and application date of mineral nitrogen as well as the fertiliser form which is used to distribute the total N into NO_3 and NH_4 pools on the soil surface.

Goal oriented fertilization

If the management data contain negative values as *quantity* for an event of N fertilization, the model uses the absolute value as nitrogen goal. In this case, the actual amount of applied fertilizer is the difference between that goal and the mineral nitrogen store in the rooted soil profile. For agro1 crops there is additionally the option to relate the application date to a specific BBCH code. In this case the *value* item in the management tab (*amount* field in table *cdy_madat*) should contain a negative number. The fertilizer will be applied at BBCH=abs(*value*).

~~Autofertilization~~

~~SBA method (German: Stickstoff-Bedarfs-Analyse)~~

~~For scenario simulations there is often no information available about the actual fertilization rates. To simulate an appropriate farming level, it is possible to calculate the required fertilizer N from the mineral N amount in the soil and the rules that are~~

~~used in advisory service for good farming practice. In CANDY, the user may apply the rules of the SBA method. In this case it is necessary to specify the dates of N application and code the amount of N with -999.~~

~~There may be up to four application dates. The first two dates are reserved to the first fertilization event. In case of too high doses, N may be split between these two dates. The next two fertilization dates belong to the second and a third fertilization event. Only for the first event the amount of N fertilizer is related to the soil storage of mineral nitrogen at that time. N amounts for the second and third event are based on table values.~~

~~Another option for auto fertilization relates to permanent grassland. The amount of N Offtake is replaced after a cutting event if the crop parameters allow for *autocut* (art=6) and *autofert* (algo=4).~~

Organic amendments

Any fresh organic matter (FOM) pool may include organic bound nitrogen as well as inorganic nitrogen. Therefore, the parameter set contains two different C/N ratios.

CNR: C_{org}/N_{org}

CNR_alt: $C_{org}/(N_{org}+N_{min})$

A third (redundant) parameter describes the relation between mineral and organic (MOR) bound N.

MOR: N_{min}/N_{org}

or

MOR: (CNR/CNR_alt) - 1

Mineralisation / Immobilisation

During FOM decomposition N is released into the ammonia pool according to the C/N ratio of the FOM pool. The FOM decomposition goes along with a microbial growth where the C reproduction flux is controlled by the η parameter of the FOM. The required N for this growth, defined by CNR_{mic}, is taken from the mineral N – first from ammonia then from nitrate. In case not enough mineral nitrogen is available and to avoid negative N_{min}, the decomposition rate is reduced.

N fixation by legume crop

Symbiotic N fixation may be an important nitrogen source especially for semi-natural systems or in case of organic farming. The process of N fixation is controlled by crop parameters containing the uptake rate from soil and the time dependence of the development of symbiotic fixation potential. After harvest the root system contains a remarkable amount of nitrogen that is handled like mineral nitrogen and distributed over the whole soil profile instead of staying only in the topsoil.

Nitrogen sinks

Plant uptake

Plant uptake is the most important sink for agroecosystems because this flux controls yield and product quality. A detailed description is given in the crop module (see Crop Module).

N losses

Leaching

NO_3-N will be leached downward with the water percolation. It is assumed that only the water in meso and macropores is moving. According to this, the nitrogen dissolved in the water of the micropores is not leached. After each leaching event the nitrogen is redistributed between the complete pore systems of each soil layer.

The leached nitrogen (N_L) from one soil layer is calculated as:

$$N_L = N_{NO_3} \cdot \left(1 - D \cdot \frac{PWP}{FC}\right) \cdot \frac{P}{\theta_0}$$

N_L	leached nitrogen	[kg ha^{-1}]
PWP	water content at permanent wilting point	[Vol. %]
FC	water content at field capacity	[Vol. %]
P	water percolation	[mm d^{-1}]
D	calibration parameter DISP_KF in CNDAPARM	[-]
θ_0	initial water content	[Vol. %]
N_{NO3}	amount of nitrate N in the calculation layer	[kg ha^{-1}]

Gaseous Losses

Ammonia volatilization is calculated at the application event of organic amendments. If no soil tillage is registered during the next 3 days, 20% of the applied NH_4-N is taken from the soil as volatilization loss.

While gaseous losses from nitrate N are calculated due to anaerobic turnovers, the temperature impact (r_T) on the anaerobic turnover is considered the same as for the BAT calculation. The following reduction function (R_θ) is applied for the soil moisture impact:

$$R_\theta = \min\left(1, \sqrt{\frac{\theta + 0.627 \cdot FC - 0.0267 \cdot LPV \cdot FC}{1.627 \cdot FC - 0.0267 \cdot LPV \cdot FC}}\right)$$

R_Θ	reduction function for soil moisture impact on denitrification	[-]
FC	water content at field capacity	[Vol. %]
LPV	limited soil pore volume; LPV=min(60,PV)	[Vol. %]
Θ	water content	[Vol. %]

The amount of volatized nitrogen (N_{deni}) is dependent on the rate constant k_{deni}, the size of the NO_3 pool (N_{NO3}), and the amount of carbon in the AOM pool (C_{AOM}). The denitrification rate is limited according to the parameter MAXDENI in CNDAPARM.

$$N_{deni} = MIN(MAXDENI, k_{deni} \cdot R_\Theta \cdot R_T \cdot N_{NO3} \cdot C_{AOM})$$

N_{deni}	denitrified nitrogen	[kg ha^{-1}]
k_{deni}	constant denitrification factor	[-]
R_Θ	reduction function for soil moisture impact on denitrification	[-]
R_T	reduction function for soil temperature impact on denitrification	[-]
MAXDENI	maximum amount of denitrification	[kg ha^{-1}]
C_{AOM}	total C amount of active organic matter	[kg ha^{-1}]
N_{NO3}	amount of nitrate N in the calculation layer	[kg ha^{-1}]

Following the approaches of Parton the N flux from denitrification is split between N_2 and N_2O (Parton et al. 1996). This partitioning is controlled by factors depending on the water filled pore space (f_{wfps}), the CO_2 production rate P_{CO2} (f_{CO2}) and the nitrate concentration C_{NO3} (f_{NO3}).

$$f_{wfps} = \frac{1.4}{13^{\left(\frac{17}{13^{(2.2 \cdot wfps)}}\right)}} \quad \text{with} \quad wfps = \frac{\theta}{PV}$$

$$f_{CO_2} = 13 + \frac{30.78 \cdot arctan\left(\pi \cdot 0.07\left(P_{CO_2} - 13\right)\right)}{\pi}$$

$$f_{NO_3} = 25 \cdot \left(1 - \left(0.5 + \frac{arctan\left(\pi \cdot 0.01\left(C_{NO_3} - 190\right)\right)}{\pi}\right)\right)$$

The partitioning coefficient $R_{N2/N2O}$ is calculated from the product of *f_wfps* and the geometric mean of the factors for NO_3 and CO_2 effects:

$$R_{N_2/N_2O} = f_{wfps} \cdot \sqrt{(f_{NO_3} \cdot f_{CO_2})}$$

Finally, the resulting N_2O flux (N_{N2O}) is calculated with:

$$N_{N_2O} = \frac{N_{deni}}{1 + R_{N_2/N_2O}}$$

Turnover of mineral nitrogen

Mineral nitrogen in soil is available as nitrate or ammonium. During the FOM decomposition ammonium will be released that in a second step is transformed into nitrate. This nitrification process is modelled assuming a Michaelis Menten kinetics:

$$\Delta N_{NH_4} = min\left(N_{NH_4}, hn \cdot \frac{NIT1 \cdot \rho \cdot N_{NH_4} \cdot BAT}{NIT2 \cdot \rho + N_{NH_4}}\right)$$

ΔN_{NH4}	is the daily nitrification rate in a given soil layer	
N_{NH4}	ammonium nitrogen in a given soil layer	[kg ha^{-1}]
BD	bulk density in a given soil layer	[g cm^{-3}]
BAT	biologic active time of the day in a given soil layer	
NIT1	Factor for nitrification control (default =40)	[kg ha^{-1}]
NIT2	Factor for nitrification control (default=90)	[kg ha^{-1}]
N_{NO3}	amount of nitrate N in a given soil layer	[kg ha^{-1}]

The constants NIT1 and NIT2 control the process if no inhibitor is applied (*hn*=1) which is the standard assumption. Other than default values are applied if nit1 and/or nit2 appear in the *cdyaparm* table.

CANDY has currently no explicit option to apply nitrification inhibitors. Therefore, this can only be activated using a sort of 'backdoor' mechanisms in versions after 22.7.10. The time dependence of *hn* is modelled using the 'S-shape' function known from N-uptake by crop where the time parameter t is steadily increased after the application date and the parameter V is extracted from the *item_ix* of the applied fertilizer (V=item_ix-500). S is set to 2 but can be overwritten by the value of *HNIT* if it is included in table *cdyaparm*.

Model output

Model outputs related to observations or results, as described in the following chapters, can be designed in a quite flexible way by means of user-created lists of the required elements as shown in Figure 24 and Figure 25. Each item in *cdy_prop* or *cdy_rslt* is represented by an object that includes the memory-address of the related feature as well as the method to produce the actual value as sum or average.

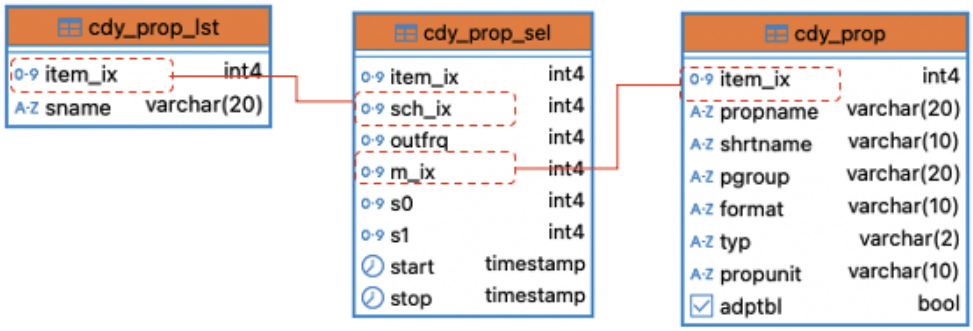


Figure 24: data structure for observation lists

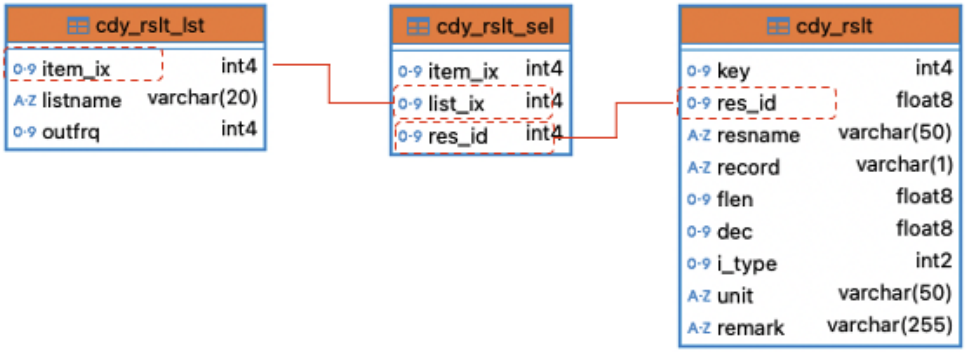


Figure 25: data structure for result lists

Observation handling

Generally, there are three types of observations that are handled at runtime:

(i) data that should be compared to model output.

(ii) data that should be used to change state variables to improve model initialization.

(iii) data records that should be filled with model results without real measurements.

While the first two types are written in table *cdy_mvdat*, the third type is generated before the model starts from the selected observation scheme and written together with the 'real' observation of the first two types into table *cdy_msdat*. For a better access, this table is ordered according to an index built from fname, snr, utlg, year,

day, mix, upper, and lower depth. This should be kept in mind if the simulation scenario is not created with the internal routines but built manually.

When the observation module is called in the *daystep* routine, it compares the first record of *cdy_msdat* with the current date. If there is a match, it is checked if the required observation (m_ix) is known and then handled according to the required mode (adapt state or report value). Afterwards, we skip to the next record.
All 'known' observations are stored in a list that is always re-created at runtime.
Remark: Most items and especially those that are expressed as concentration are related to *fine* soil if stone content is considered the item has the postfix '_stc'.

The definition of observation items is dynamical in the sense that the table cdy_prop is generated by the program. This gives the option to define new observation items with an update of the model software.
The definition of each observation item includes all elements of cdy_prop , a label for the reference object that represent the basic address and up to three offset numbers that are used to calculate the address of the required variable.
Example to calculate N_{min} in fine soil:
The state record of candy contains two arrays (type *profile*) with the amount of both N forms nitrate (*nin*) and ammonium N (*amn*) both in kg/ha in each calculation layer. To get the total amount of mineral nitrogen from layer i to layer j all numbers of *nin* and *amn* in this range have to be added. This job is done by a generic procedure that is used for all variables of type profile.
To get the address of the variables we have to add the offset values to the address of the base :

```
p:=pointer(NativeUInt(lobs.aobs.base_obj)+ lobs.aobs.info.offset);
```

Then, a local variable x of type *profile* is located on this address:

```
x:=profil(p2^);
```

and finally the sum can be calculated

```
v:=0
for i:= lobs.avon+1 to lobs.abis do v:=v+x2[i];
```

This is repeated, if more offset values are provided.

The offset values itself are calculated during initalisation like shown in the following example for candy (this is the model kernel). as base object:

```
offset := NativeUInt(@candy.s.ks.nin)-NativeUInt(@candy);
```

The addresses (given by the @ operator) have to be transformed into the native integer format of the system (MacOS or Win) to get the correct result. Knowing the address of the required variable the value can be reported as s_wert or it may be changed according to the given value in m_wert if adaptation is required and the variable has the potential to be adapted. So, the adaptation of Nmin, for instance, at the beginning

of the simulation can improve the initialization but obviously there is no sense in changing flux values like N2O production.

The list of available observation items depends on the model version and may be updated in future.

Here is an overview of the currently available properties for observation handling:

mix	name	short	group	unit	adapt-able	comment
0	SoilTotalNitrogen	Nt_conc	SOM	M%	true	
2	decomposable SOC	SOC_dec	SOM	kg/ha	false	
6	hotwater soluble C	C_HWS	SOM	mg/100g	false	
7	SoilOrganicCarbon	Corg_conc	SOM	M%	true	
23	CrepFlx	CrepFlx	SOM	kg/ha/d	false	
28	SOC_stock_stc	SOC_stock_	SOM	kg/ha	true	
51	CinMulchLayer	C_Mulch	SOM	kg/ha	false	
202	decomposableSOC_stc	SOC_dec_st	SOM	kg/ha	false	
18	dailyNPP	dNPP	crop	kg	false	
19	transkoeff	transko	crop	mm	false	
20	N_yield	N_yield	crop	kg/ha	false	
21	NatYld-Byp	NatYldByp	crop	dt/ha	false	
22	NatYld-MP	NatYldMP	crop	dt/ha	false	
26	DM-Yld-Mp	DMYldMp	crop	dt/ha	false	
27	DM-Yld-ByP	DMYldByP	crop	dt/ha	false	
29	N-Yld-Mp	NYldMp	crop	kg/ha	false	
30	N-Yld-ByP	NYldByP	crop	kg/ha	false	
31	C-Yld-Mp	CYldMp	crop	kg/ha	false	
32	C-Yld-ByP	CYldByP	crop	kg/ha	false	
35	crop DC state	crop DC	crop	-	false	
36	ActDM_MP	aDM_MP	crop	kg/ha	false	
37	ActDM_ByP	aDM_ByP	crop	kg/ha	false	
45	ActRootDpth	actRtDpth	crop	dm	false	
46	ActCropCover	actCover	crop	-	false	
49	LeafAreaIndex	LAI	crop	-	false	
56	N upt from layer	Nupt_Lay	crop	kg/ha	false	
57	W upt from layer	Wupt_Lay	crop	mm	false	
59	ActDM_crop	aDM_crop	crop	kg/ha	false	
69	YldNofftake	YldNoff	crop	kg/ha	false	
8	soil water_stc	soil_w_stc	environment	mm	false	
9	soil temperature	soil_temp	environment	°C	true	
10	SoilMoisture(VOL)	soilmoistV	environment	VOL%	true	
11	SoilMoisture(M)	soilmoistM	environment	M%	false	
24	seepage to groundw	GW_seep	environment	mm	false	
25	transpiration	transp	environment	mm	false	
47	PotEvapTransp	PET	environment	mm	false	
48	corrected Rain	corRain	environment	mm	false	
52	BiolActTime	BAT	environment	d	false	
53	act.EvapoTransp	AET	environment	mm	false	
54	water flux from laye	Wflux_Lay	environment	mm	false	
70	DrainWaterFlow	drainW	environment	mm	false	
99	el_resistivity	elRes	environment	S	false	
1	nitrate N	NO3_N	nitrogen	kg/ha	true	
3	amonium N	AMN_N	nitrogen	kg/ha	true	
4	mineralN	MIN_N	nitrogen	kg/ha	false	
44	mineralNconc	MIN_N_C	nitrogen	mg/kg	false	
50	NinMulchLayer	NtMulch	nitrogen	kg/ha	false	
55	Nit.N.Conc	NO3N_Conc	nitrogen	mg N/L	false	
58	N flux at layer	Nflux_Lay	nitrogen	kg/ha	false	
72	DrainNitFlow	drainN	nitrogen	kg/ha	false	
75	N2O_N	N2OLoss	nitrogen	kg/ha/d	false	

76	NGasLoss	NGasLoss	nitrogen	kg/ha/d	false	
204	mineralN_stc	MIN_N_stc	nitrogen	kg/ha	false	
61	field capacity	FieldCap	structure	cm3/cm3	false	
62	perm. wilting point	PWP	structure	cm3/cm3	false	
63	bulk density	BD	structure	g/cm3	false	
64	particle density	PD	structure	g/cm3	false	
65	pore volume	P_VOL	structure	cm3/cm3	false	

Result processing

Other than observation outputs, result recording is less flexible. Users can only select a fix time schema for output and can only select between the predefined result options without modification of depth. If required, the time schema can be extended to also include the harvest dates, setting the switch *rs_at_hrv*=1 in the ini file. If this switch is on, the yield results are written into the result table without explicitly selecting an yield related item.
Technically, the access to state variables for result recording is like the methodology for observation results. But other than observations, some results can be accumulated during simulation, depending on their definition. Like the processing of observations, the result recording is prepared during model initialization using the required result list containing a free selection of result items and the required time interval. The possible time intervals are:

Days	(1)
Pentade (five days)	(2)
Decade (ten days)	(3)
Months	(4)
Years	(5)

The numbers shown in parentheses are accepted values for res_out in table *cdy_rslt_lst* (Figure 25)

When the result module is called in the *daystep* routine, it will decide if an output is required or not and process the complete list of required results calling their individual *get_value* and *update* methods and eventually also the *put_value* method that will continue the defined result table (*rs_...*).

Access to results is controlled by the result numbers and model updates may provide new options. Here is the current state:

res_nr	result name	unit	type	remark
90	C_AOS	dt/ha	0	C in AOS (0-30cm)
91	C_SOS	dt/ha	0	C in SOS (0-30cm)
92	CDEC	kg/ha	0	Decomposable SOC (0-30cm)
93	COPS	kg/ha	0	C in all FOM pools
95	CLTS	kg/ha	0	Long term Stabilised SOC (0-30cm)
96	SOC_SEQ	kg/ha	0	SOC sequestration (0-30cm)
100	NIED_K	mm	1	Corrected (effective) rainfall.
101	WBIL	mm	1	Climatic water balance

102	N_leach	kg/ha	1	N-leaching
103	GWB	mm	1	Ground water recharge
104	BAT	d	1	Biol.Act.Time
105	SRO	mm	1	surface runoff
106	N_gfv	kg/ha	1	gaseous. N-lossese
107	N_MIN_S	kg/ha	1	N-Mineralization
108	BW_0_3	mm	0	Soil water 0-30cm
109	BW_0_10	mm	0	Soil water 0-100cm
110	BT_0_3	°C	2	Soil temperature 0-30cm
111	N_OBFL	kg/ha	0	N on soil surface
112	NMIN_0_3	kg/ha	0	Nmin 0-30cm
113	NMIN_3_6	kg/ha	0	Nmin 30-60cm
114	NMIN_6_10	kg/ha	0	Nmin 60-100cm
115	BW_PRFL	mm	0	Soil water(0-smax)
116	NMIN_PRFL	kg/ha	0	Nmin (0-smax)
117	N_OPS	kg/ha	0	N in all FOM pools
118	N_OBS	kg/ha	0	N in all SOM pools
119	NI_MIN	kg/ha	1	N Input from mineral sources
120	NI_ORG	kg/ha	1	N Input with organic matter
121	NI_SYM	kg/ha	1	N Input from symbiotic fixation
122	N_UPT	kg/ha	1	N-uptake by crop
123	NH4VT	kg N/ha	1	Gaseous NH4-loss
124	NSUMSYS	kg/ha	0	Total N in system
125	N_M_SUMSYS	kg/ha	0	Total N-min in system
127	M_BEDGRD	-	2	plant cover degree
128	NIED	mm	1	rainfall
129	PET_SUM	mm	1	potential evapotranspiration.
130	S_TRANSP	mm	1	Transpiration
135	C_REP_SUM	kg/ha	1	C-REP-Flux
136	C2M	kg/ha	0	Carbon flux into mulch
137	NPP	g/m²	1	NetPrimaryProduction
138	NEE	g/m²	1	NetEcosystemExchange
139	C_MIN	kg/ha	1	C-Mineralization
140	WSAS	mm	0	Water storage above soil
141	LTEMP	°C	2	Air temperature
142	AET_SUM	mm	1	actual evapotranspiration
143	WDF	mm	1	Water flux into drainage
144	NDF	kg/ha	1	Nitrogen flux into drainage
145	N-deposition	kg/ha	1	N-Deposition
146	GLOB	MJ/m²	2	Global Radiation
147	SRFEVP_SUM	mm	1	Water evaporation from surface.
150	Auto_BW	mm	0	Automatic Irrigation
201	N_off_crop	kg/ha	1	N-Offtake by Crop
202	N_upt_crop	kg/ha	1	N-Uptake by Crop
203	Nupt_BPR	kg/ha	1	by-product: N-Uptake

204	Nupt_CrRes	kg/ha	1	crop residues: N-Uptake
701	DD_AP_val (SSD)	g/cm³	2	DD_AP_val (SSD)
704	TRD_30 (SSD)	g/cm³	2	Soil bulk density 0-30 cm (SSD)
705	FCAP_30 (SSD)	VOL%	2	Field capacity 0-30 (SSD)
706	PWP_30 (SSD)	VOL%	2	Perm. wilting point 0-30cm (SSD)
707	PVOL_30 (SSD)	VOL%	2	Pore volume 0-30cm (SSD)
997	N2O	kg/ha	1	N2O-emission

Pedotransferfunctions in CANDY

Modelling of processes and turnover in agro ecosystems requires detailed information about the soil and soil water balance. Since measurements of soil physical parameters are time consuming and expensive, application of pedotransfer functions (PTF) is an appropriate alternative. This enables the estimation of required soil properties (e.g., field capacity, permanent wilting point) from other known and easily measurable properties (e.g., texture). Furthermore, the implementation of the dynamical description of soil structure in CANDY bases on the application of PTFs (e.g., bulk density) (see chapter Soil structure dynamics).

Soil texture class conversion

In some approaches the soil texture is based on the USDA7 system. This system defines clay as the particle size fraction < 2 µm, silt as the fraction between 2 and 50 µm and sand as the fraction between 50 and 2000 µm. For converting the German soil system into the USDA7 system, the following interpolation after Nemes et al. (1999) is useful:

$$y = (y_2 - y_1) \cdot \frac{log(x) - log(x_1)}{log(x_2) - log(x_1)} + y_1$$

STX	soil texture class	[M. %]
x	particle size diameter of the missing y (upper limit)	[mm]
y	cumulative percentage on the particle-size distribution curve with particle size diameter x	[M. %]
y_1	cumulative percentage on the particle-size distribution curve with the next small particle size diameter	[M. %]
y_2	cumulative percentage on the particle-size distribution curve with the next bigger particle size diameter	[M. %]
x_1, x_2	corresponding particle size diameters to y_1 and y_2	[mm]

Bulk density

The dynamic of bulk density (BD) is described in chapter Soil structure dynamics. If only clay content and C_{org} content are available, it is possible to calculate bulk density using the approach of Körschens (1980) (see: Ruehlmann and Körschens (2009)):

$$BD = 1.64 - 0.0075 \cdot T - 0.0611 \cdot C_{org}$$

Particle density

The particle density PD is calculated following an approach depending on actual C_{org} given by Rühlmann et al. (2006).

$$PD = \left(\frac{Q_{OS}}{\rho_{OS}} + \frac{1-Q_{OS}}{\rho_{min}}\right)^{-1} \text{ with } \rho_{OS} = 1.127 + 0.373 \cdot Q_{OS} \text{ and } Q_{OS} = \frac{C_{org}}{55}$$

Q_{OS}	volumetric part of organic matter	[-]
C_{org}	soil organic carbon concentration	[M. %]
ρ_{OS}	density of organic matter	[g cm^{-3}]
PD	particle density	[g cm^{-3}]
ρ_{min}	density of mineral substance (site specific parameter)	[g cm^{-3}]

Pore Volume

The pore volume is based on the relation between bulk density (BD) and particle density (PD).: $PV = 1 - \mathrm{BD/PD}$

Hydraulic parameters according to Lieberoth

The simplest approach to calculate field capacity and permanent wilting point after Lieberoth (1982) is based on soil texture data only.

$$\mathrm{FC} = 3.4 + 0.85 \cdot \mathrm{ABT}$$

$$\mathrm{PWP} = 1.23 + 0.74 \cdot \mathrm{T}$$

FC	water content at field capacity	[mm]
ABT	particles < 20 µm	[M. %]
PWP	permanent wilting point	[mm]
T	clay content (< 2 µm)	[M. %]

Water retention model according to van Genuchten

$$\theta(\psi) = \theta_r + \frac{\theta_s - \theta_r}{(1+(\alpha \cdot |\psi|)^n)^m}$$

α	van Genuchten parameter	[cm^{-1}]
n	van Genuchten parameter	[-]
m	van Genuchten parameter	[-]
ψ	matric potential	[hPa]
θ_r	residual water content	[0..1]
θ_s	saturation water content	[0..1]

Approach of Vereecken

Vereecken et al. (1989) calculated the van Genuchten parameters using USDA7 texture classes :

$$\theta_s = 0.81 - 0.283 \cdot BD + 0.001 \cdot T$$
$$\theta_r = 0.015 - 0.005 \cdot T + 0.014 \cdot C_{org}$$
$$\alpha = e\exp(-2.486+0.025 \cdot S - 0.351 \cdot C_{org} - 2.617 \cdot BD - 0.023 \cdot T)$$
$$n = e\exp(0.053 - 0.009 \cdot S - 0.013 \cdot T + 0.00015 \cdot S^2)$$
$$m = 1$$

Approach of Zacharias & Wessolek

Zacharias and Wessolek (2007) calculated the Van Genuchten parameters without using the organic carbon content based on USDA7 texture classes.

For S < 66.5

$$\theta_s = 0.788 - 0.263 \cdot BD + 0.001 \cdot T$$
$$\theta_r = 0$$
$$\alpha = e(-0.648+0.023 \cdot S - 3.168 \cdot BD - 0.044 \cdot T)$$
$$n = 1.392 + 1.212 \cdot T^{-0.704} - 0.418 \cdot S^{-0.024}$$
$$m = 1 - 1/n$$

For S ≥ 66.5

$$\theta_s = 0.89 - 0.322 \cdot BD + 0.001 \cdot T$$
$$\theta_r = 0$$
$$\alpha = e(-4.197+0.013 \cdot S - 0.276 \cdot BD - 0.076 \cdot T)$$
$$n = -2.562 + 3.75 \cdot T^{-0.016} + 7 \cdot 10^{-9} \cdot S^{4.004}$$
$$m = 1 - 1/n$$

T : clay content. [M. %]

S : sand content [M. %]

BD: bulk density [g cm^{-3}]

HYPRES approach

$$\theta_s = 0.7919 + 0.001691 \cdot T - 0.29619 \cdot BD - 0.000001491 \cdot S^2 + 0.0000821 \cdot OM^2 + 0.02427/T + 0.01113/S + 0.01472 \cdot ln(S) - 0.0000733 \cdot OM \cdot T - 0.000619 \cdot BD \cdot T - 0.001183 \cdot BD \cdot OM - 0.0001664 \cdot S$$

$\theta_r = min(0.25, 0.01 + 0.0048 \cdot SC)$ *(adapted for continuous change with stone content)*

$$\alpha = \exp(-14.96 + 0.03135 \cdot T + 0.0351 \cdot S + 0.646 \cdot OM + 15.29 \cdot BD - 0.192 - 4.671 \cdot BD^2 - 0.000781 \cdot T^2 - 0.00687 \cdot OM^2 + 0.0449/OM + 0.0663 \cdot ln(S) + 0.1482 \cdot ln(OM) - 0.04546 \cdot BD \cdot S - 0.4852 \cdot BD \cdot OM + 0.00673 \cdot T)$$

$$n = 1 + \exp(-25.23 - 0.02195 \cdot T + 0.0074 \cdot S - 0.1940 \cdot OM + 45.5 \cdot BD - 7.24 \cdot BD^2 + 0.0003658 \cdot T^2 + 0.002885 \cdot OM^2 - 12.81/BD - 0.1524/S - 0.01958/OM - 0.2876 \cdot ln(S) - 0.0709 \cdot ln(OM) - 44.6 \cdot ln(BD) - 0.02264 \cdot BD \cdot T + 0.0896 \cdot BD \cdot OM + 0.00718 \cdot T)$$

$m = 1 - 1/n$

T : clay
S : usda_sand (T,U) – U limit : GER=> 0.063 ; USDA => 0.05
OM: 1.724 · C_{org}
SC: stone content (gravel) in Vol%

Further reading: Chirico et al., 2007; Wösten et al., 1999

Water retention model according to Brooks-Corey

$$\theta(\psi) = \begin{cases} \theta_r + (\theta_s - \theta_r) \cdot \left(\frac{\psi}{\psi_b}\right)^{-\lambda} & \psi < \psi_b \\ \theta_s & \psi \geq \psi_b \end{cases}$$

$\Theta(\Psi)$	water content as function of matric potential	[Vol. %]
Ψ	matric potential	[hPa]
Ψ_b	air entry potential	[hPa]
Θ_r	residue water content	[Vol. %]
Θ_s	saturation water content	[Vol. %]
λ	pore size index	[-]

Approach of Rawls and Brakensiek

Rawls and Brakensiek calculated the Brooks-Corey parameters from pore volume based on USDA7 texture classes (clay and sand fraction) (Brooks 1964, Rawls and Brakensiek 1985).

$$\Psi_b = exp(5.3396738 + 0.1845038 \cdot T - 2.48394546 \cdot PV - 0.00213853 \cdot T^2 - 0.04356349 \cdot S \cdot PV - 0.61745089 \cdot T \cdot PV + 0.00143598 \cdot S^2 \cdot PV^2 - 0.00855375 \cdot T^2 \cdot PV^2 - 0.00001282 \cdot S^2 \cdot T + 0.00895359 \cdot T^2 \cdot PV - 0.00072472 \cdot S^2 \cdot PV + 0.0000054 \cdot T^2 \cdot S + 0.5002806 \cdot PV^2 \cdot T)$$

$$\lambda = exp(-0.7842831 + 0.0177544 \cdot S - 1.062498 \cdot PV - 0.00005304 \cdot S^2 - 0.00273493 \cdot T^2 + 1.11134946 \cdot PV^2 - 0.03088295 \cdot S \cdot PV + 0.00026587 \cdot S^2 \cdot PV^2 - 0.00610522 \cdot T^2 \cdot PV^2 - 0.00000235 \cdot S^2 \cdot T + 0.00798746 \cdot T^2 \cdot PV - 0.00674491 \cdot PV^2 \cdot T)$$

$$\Theta_r = -0.0182482 + 0.00087269 \cdot S + 0.00513488 \cdot T + 0.02939286 \cdot PV - 0.00015395 \cdot T^2 - 0.0010827 \cdot S \cdot PV - 0.00018233 \cdot T^2 \cdot PV^2 + 0.00030703 \cdot T^2 \cdot PV - 0.0023584 \cdot PV^2 \cdot T$$

$$\Theta_s = 0.01162 - 0.001473 \cdot S - 0.002236 \cdot T + 0.98402 \cdot PV + 0.0000987 \cdot T^2 + 0.003616 \cdot S \cdot PV - 0.010859 \cdot T \cdot PV - 0.000096 \cdot T^2 \cdot PV - 0.002437 \cdot PV^2 \cdot S +$$

$$0.0115395 \cdot PV^2 \cdot T$$

Θ_r	residue water content	[Vol. %]
Θ_s	saturation water content	[Vol. %]
Ψ_b	air entry point	[hPa]
λ	pore size index	[-]
T	clay content	[M. %]
S	sand content	[M. %]
PV	pore volume (as relative number)	[0..1]

Usage in CANDY:

Switching between the different pedotransfer functions for the hydrologic parameters can be done changing ptfmode in the ini file:

ptfmode = 1 for Rawls Brakensiek/Brooks-Corey

ptfmode = 2 for Vereecken/van Genuchten (recommended standard)

ptfmode = 3 for Lieberoth

ptfmode = 4 for Zacharias/van Genuchten

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