CANDY Manual

Description of Background

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Model description

Introduction

The agro-ecosystem model CANDY (Carbon And Nitrogen DYnamics) has been developed to describe carbon and nitrogen dynamics in arable soils in order to provide information about carbon stocks in soils, organic matter turnover, nitrogen uptake by crops, leaching and water quality.

It consists of a modular system of sub models and a data base system for model parameters, initial soil values, weather data, soil management data and measurement values. The user interface of the model provides geographic information system facilities that are designed to organize regional scenario simulations.

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

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

Special features are:

- CANDY 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.
- An optional auto fertilizer scheme (SBA) implements good farming practices for mineral nitrogen application.
- The optional CIPS approach describes the relevance of soil structure for the long term stabilization of soil organic matter.

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 a number of projects and with the input of many people more and more adjustments have been made in order to make the model usable for the specific task. Now we speak about CANDY as a system consisting of a number of modules where some of them are mandatory for ecosystem modelling because they provide the infrastructure and other may be switched on or off depending on the objective and the available data. There are for instance different modules for crop dynamics and for SOM turnover as well.

To make things more complex the modules may have different parameters. Because of this reason any user has to develop a clear idea about the objective of the modelling work and the required database. It is necessary to check the available parameter tables if they contain already the required information.

The CANDY infrastructure covers the main processes that are relevant for an agro-ecosystem and the required facilities for the data management:

Access to soil properties

Soil is in the main focus of 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 one dimensional profile consisting of separate horizons that are mainly characterized by soil texture and a set of soil physical properties. In contrast to natural horizon dimensions the model regards 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 dynamics.

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 fertilization, adding of organic matter and water input. Each tillage operation leads to averaging of the state variables of the affected calculation layers.

Access to measurement data

All measurement data are stored within a specific table. During the preparation of a simulation run all or selected data are temporarily moved to another table 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 an user interface. In some cases (e.g. 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 user that have no separate software for database management available.

Generation of result records

Beside the interface to the measurements users may select a number of predefined results in an appropriate time resolution. 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.

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 single modules may be different. Some are used with good results over many years and other are rather new with only limited results.

Description of process modules

The following chapters present the currently available modules. Each chapter is starting with an overview about the inputs, outputs and parameters, including the source of the parameter, its measurement id that can be find in the table CND_MWML as well as the result id from table CDY_RSLT. This part is then followed by description of the algorithms used.

Soil temperature dynamics

Input

symbol	description	unit	source
T_{air}	daily mean air temperature	[°C]	CDY_CLDAT
Ɵ	soil moisture	[Vol. %]	Internal

Output

symbol	description	unit	measurement id	result id
T_s	soil temperature	[°C]	9	110 (0-3 dm)

Parameters

symbol	description	unit	source
HKAP	specific heat capacity of the dry soil	[J cm^{-3} K^{-1}]	CNDHRZN
α	thermal conductivity (const.)	[J s^{-1} cm^{-1} K^{-1}]	Internal
AMP	amplitude	[°C]	CDYBTPRM
PHA	phase shift of the sinus/cosinus function	[d]	CDYBTPRM
LTEM	mean annual air temperature	[°C]	CDY_FXDAT

Description

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

The soil temperature influences the soil water viscosity and thereby the water fluxes within the profile. The influence on the C/N turnover in the model is considered by a reduction function during calculating the Biological Active Time (see chapter 3.3).

The state variable of the temperature module is the soil temperature (T_s). It is modelled by solving the heat flow equation after Suckow (1987) (Equation 1).

$$\frac{\partial(HKAP \cdot T_s)}{\partial t} = \frac{\partial}{\partial z}\left(\alpha \frac{\partial T_s}{\partial z}\right) \tag{1}$$

t	time	[d]
z	depth	[cm]
HKAP	specific heat capacity of moist soil	[J cm^{-3} K^{-1}]

| T_s | soil temperature | [K] |
| α | thermal conductivity of moist soil | [J s^{-1} cm^{-1} K^{-1}] |

Two boundary conditions for Equation 1 have to be given. The upper boundary of soil temperature (at 5 cm depth) is defined as the weighted mean of the air temperatures of the present day, yesterday and the day before yesterday, multiplied by a time-dependent correction factor. The correction is done in order to take into account the neglected meteorological elements and for the crop influence on surface temperature.

As the lower boundary condition (zero heat flow) is assumed at a depth of 200 cm. The soil temperature distribution within the profile is calculated using the air temperature and the lower boundary condition. The soil temperature at 200 cm is calculated depending on the season of the year, either summer (120 < Julian day < 304, Equation 2) or winter (Equation 3).

Lower boundary (summer):

$$d_S = AMP \cdot \sin\left[(dnr + PHA) \cdot \frac{2\pi}{365}\right] + LTEM \tag{2}$$

d_s	daily soil temperature in summer time	[°C]
AMP	amplitude	[°C]
sin	sinus function	
dnr	Julian day	
PHA	phase shift of the sinus function	[d]
π	Pi	
LTEM	mean annual air temperature	[°C]

Lower boundary (winter):

$$d_W = AMP \cdot \cos\left[(dnr + PHA) \cdot \frac{2\pi}{365}\right] + LTEM \tag{3}$$

d_w	daily soil temperature in winter time	[°C]
AMP	Amplitude	[°C]
cos	cosinus function	
dnr	Julian day	
PHA	phase shift of the cosinus function	[d]
π	Pi	
LTEM	mean annual air temperature	[°C]

In order to fit simulated to measured data, the parameters AMP and PHA (table CDYBTPRM) can be calibrated. The mean air temperature (LTEM from table CDY_FXDAT) has an influence as well, according to the summer or winter period. The parameters AMP, PHA and LTEM should be fitted to the temperature curve of several years (Figure 1).
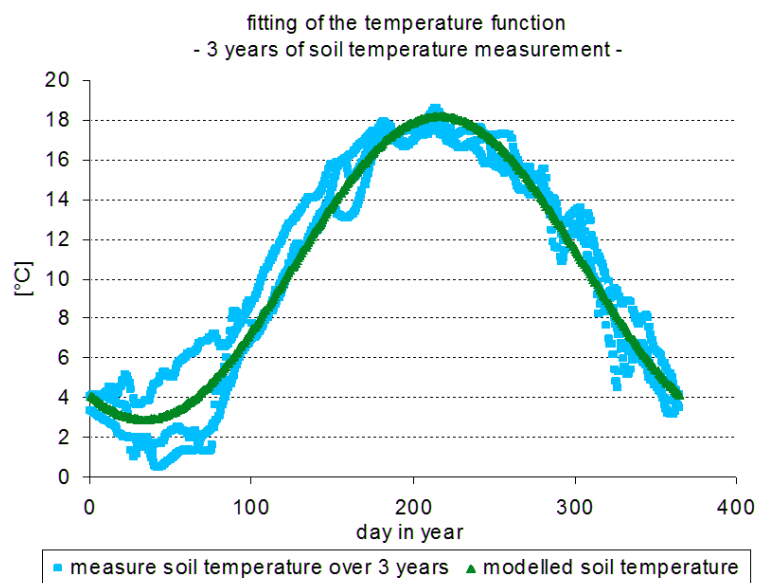
fitting of the temperature function
- 3 years of soil temperature measurement -

■ measure soil temperature over 3 years ▲ modelled soil temperature

Figure 1: Fitted soil temperature function to observed data over 3 years

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

Output

symbol	description	unit	measurement id	result id
Θ	water content of a soil column of defined thickness	[mm]	10 (Vol. %) 11 (M. %)	108 (0-3 dm) 115 (profile)
Q	drainage	[mm]	16 (profile) 54 (soil layer)	103 (profile)
ET_p	potential evapotranspiration	[mm d^{-1}]	47	129
ET_a	actual evapotranspiration	[mm d^{-1}]	19	142

Parameters

symbol	description	unit	source
FC	water content at field capacity	[Vol. %]	CNDHRZN
PWP	permanent wilting point	[Vol. %]	CNDHRZN
λ	drainage parameter	[mm^{-1} d^{-1}]	CNDHRZN
FAT	clay and fine silt (particles ≤ 6.3 μm)	[M. %]	Internal
ABT	elutriable particles < 20 μm	[M. %]	CNDHRZN
K_s	saturated hydraulic conductivity	[mm^{-1} d^{-1}]	CNDHRZN
h_{pl}	crop height	[cm]	Internal
BG	fraction of the soil surface covered by plants	[0..1]	Internal

Description

The state of water in soil is described in terms of the amount of water and the energy associated with the forces which hold the water in the soil. The amount of water is defined by water content and the energy state of the water is 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 water in soil 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 all natural systems, 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 water and soil are less than the gravitational forces acting on the water molecule and water moves downward. The matrix arrangement of soil solid particles determines the soil water matric potential. The magnitude of the forces depends on 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 curves) between water content and water potential for each soil (Figure 2).
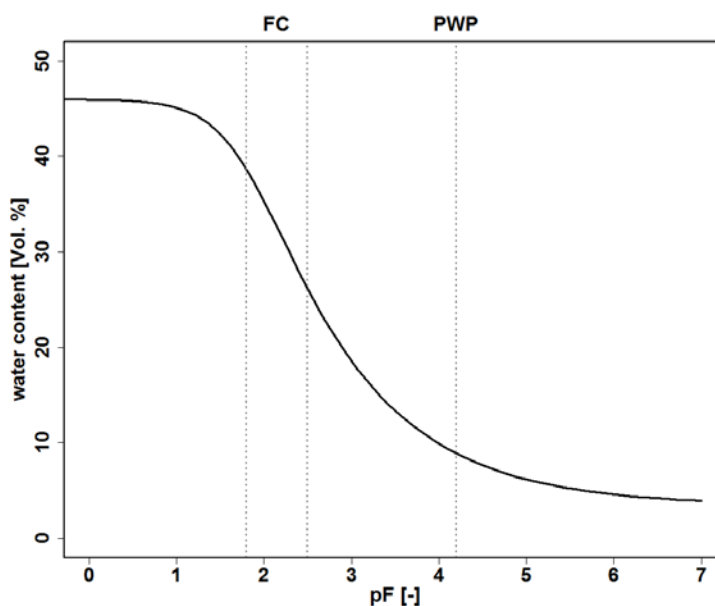
Figure 2: Water content dependencies from logarithmic matric potential (pF) exemplarily for a silt soil

The CANDY water module describes the relevant processes of water flux in the unsaturated zone (Figure 3) of soils using calculation layers of 1 dm depth. CANDY is a 1 dimensional model thereby lateral fluxes are not considered. Surface runoff occurs as a result of an infiltration surplus if the precipitation water cannot longer enter the pore system of the soil.

The CANDY model uses the capacity concept as standard concept for calculating water flux in the soil/water movement.

Downward flow of infiltrated water is only allowed if water storage exceeds a soil and horizon specific value of field capacity (Figure 4). Initial conditions can be defined by the user via the model interface. Initial values can be defined for each layer by observation data or for the entire soil profile as a given percentage of water filled pore space up to the field capacity.

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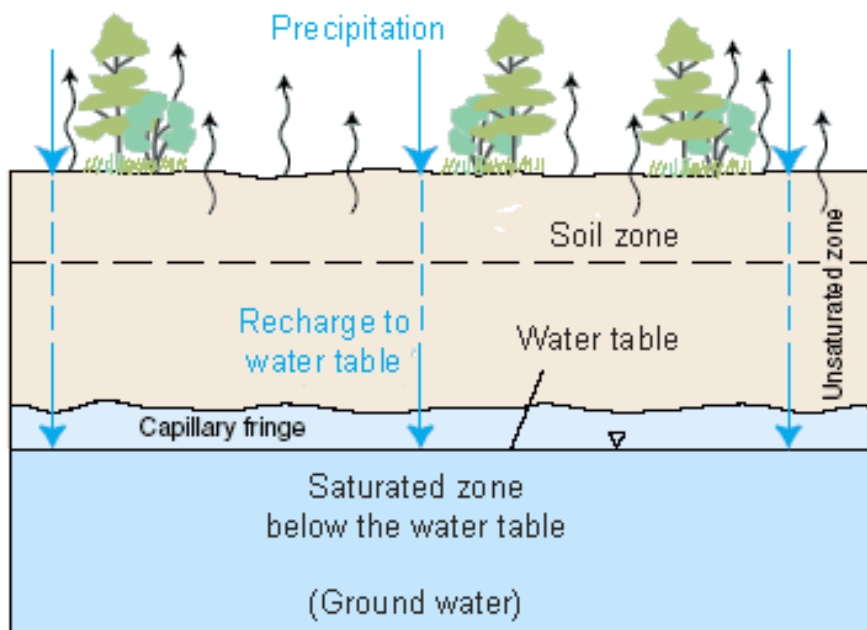
Figure 3: Relevant processes of water flux in the unsaturated zone described by the CANDY water module (http://water.usgs.gov/edu/watercycleinfiltration.html)

Soil specific parameters of the water module can be defined within the soil profile description (CNDHRZN).
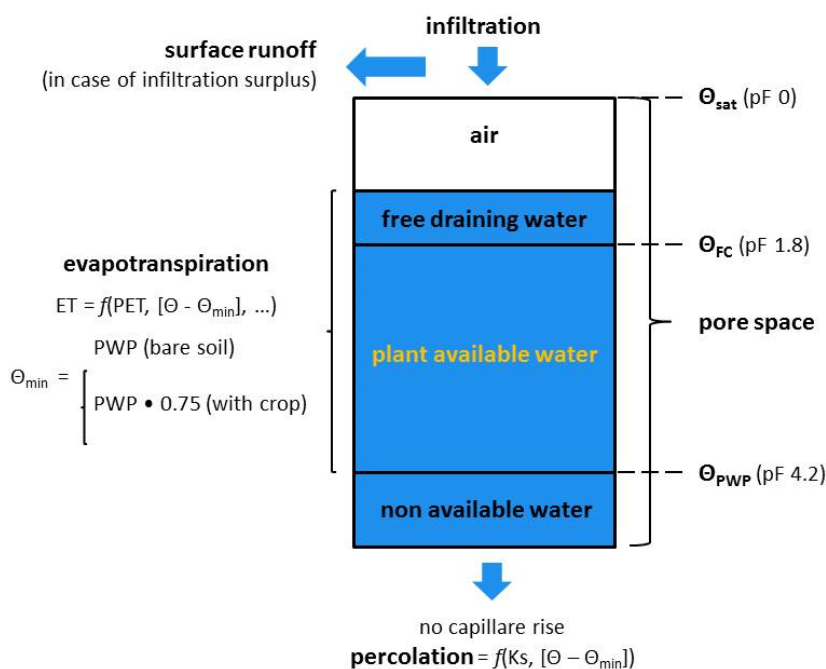
Figure 4: Soil water dynamics described within the CANDY water module for a horizon of defined thickness

Percolation

The velocity of the downward flow (Equation 4) is controlled by the saturated hydraulic conductivity through the drainage parameter (λ) (Glugla 1969, Koitzsch 1990).

$$\frac{d\Theta}{dt} = \lambda \cdot (\Theta - FC)^2 \qquad (4)$$

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

If the actual water content is lower than the field capacity, no percolation is possible. The drainage (Q) of each horizon is calculated (Equation 5).

$$Q = \frac{\lambda \cdot (\Theta - FC)^2}{[1 + \lambda \cdot (\Theta - FC)]} \qquad (5)$$

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

The drainage parameter (λ) is internal calculated from the saturated conductivity (K_s) (Equation 6).

$$\lambda = \frac{0.01 \cdot K_s}{PV - FC} \qquad (6)$$

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) (Equation 7 and Equation 8).

$$\lambda = 1.6 - 0.1565 \cdot ABT + 8.424 \cdot 10^{-3} \cdot ABT^2 - 2.551 \cdot 10^{-4} \cdot ABT^3 \qquad (7)$$
$$+ 4.28 \cdot 10^{-6} \cdot ABT^4 - 3.625 \cdot 10^{-8} \cdot ABT^5 + 1.207 \cdot 10^{-10} \cdot ABT^6$$

with: $ABT = T + fU + mU$ $\qquad (8)$

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	[mm^{-1} d^{-1}]

If water storage exceeds the pore volume of a calculation layer the amount surplus water is added to the calculation layer above. If the soil surface is reached the soil water is considered as runoff or puddle. The maximum water storage of the puddle (MPH) is calculated in mm (Equation 9).

$$MPH = 40.667 + 0.592 \cdot FC_{upper\_layer} \tag{9}$$

Interception

The interception of water by a crop (Equation 10) depends on the crop height (Koitzsch 1990, Koitzsch and Günther 1990).

$$C_i = 2.5 \cdot BG \cdot h_{pl} \tag{10}$$

C_i	interception capacity	[mm]
h_{pl}	crop height	[cm]
BG	fraction of the soil surface covered by plants	[0..1]

Snow accumulation and melting

The process of snow accumulation and melting is calculated according to Koitzsch (1990): snow fall is only possible if rainfall occurs and mean daily temperature is ≤ 0.5 °C. Melting and infiltration can occur during mean daily temperature > 0.5 °C.

Evapotranspiration

Evapotranspiration in the CANDY water module is allowed if water storage exceeds a soil and horizon specific value of minimum water content (Figure 4). The process of evaporation is calculated with a modified TURC – equation, based on the work of Koitzsch and Günther (Turc 1961, Koitzsch 1990, Koitzsch and Günther 1990). The calculation of potential evapotranspiration (Equation 11, Equation 12 and Equation 13) and actual evapotranspiration (Equation 14) is according to Koitzsch (1990).

$$ET_p = (1 + 0.004 \cdot h) \cdot E_p \; ; h \leq 100 \tag{11}$$

ET_p	potential evapotranspiration	[mm d^{-1}]
h	crop height	[cm]
E_p	value of pan evaporation	[mm d^{-1}]

with:

$$E_p = 0.0041 \cdot (T_{air} + 22.7) \cdot (G + 2.09) \tag{12}$$

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

$$EI_p = 1.3 \cdot E_p \qquad (13)$$

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

$$ET_a = 0.5 \min(EI_p, R_i) + \Psi \cdot H_1 \max\left(0, \left(1 - \frac{R_i}{EI_p}\right) \cdot ET_p\right) + (1 - \Psi) \cdot H_2 \cdot E_p \qquad (14)$$

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 funct. of water content
ET_p potential evapotranspiration   [mm d^{-1}]
EI_p potential evaporation of intercepted water by crop   [mm d^{-1}]
E_p value of pan evaporation   [mm d^{-1}]

Soil structure dynamics

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
TRD	bulk density	[g cm^{-3}]	63	704 (0-3 dm)
TSD	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}]	CDYAPARM

All other parameters are determined internally. Therefor see Equation 15 to Equation 25 in this chapter.

Description

Further enhancement of the CANDY model system is related to the integration of the CIPS model (see OM-turnover) and the implementation of a module for the dynamic description of soil structure.

Please be aware that this module is still in 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
* Particle density
* Pore volume (as defined by the both values above)
* Field capacity
* Permanent wilting point

The soil parameters have to 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 can be calculated using the Brooks-Corey approach for the water retention curve with the pedotransfer function from Rawls

and Brakensiek (1985). An alternative approach is the Van Genuchten (1980) model with the pedotransfer function from either Vereecken et al. (1989) or Zacharias and Wessolek (2007) . The detailed description of the implemented functions is given in chapter Pedotransferfunctions.

Bulk density

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) (Equation 15) occurs as a result of soil tillage, bio- and cryoturbation (Equation 20 to Equation 22). 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 (Equation 17 to Equation 19).

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

Soil loosening

$$BD_{new} = BD_{old} - ef \cdot \left(BD_{old} - \frac{2}{3} \cdot BD_0 \right) \tag{15}$$

BD_{new}, BD_{old}	bulk density	[g cm^{-3}]
BD_0	bulk density after complete re-compaction	[g cm^{-3}]
ef	loosening efficiency of soil tillage tool	[0..1]

Re-compaction

$$BD_{new} = BD_{old} + (BD_0 - BD_{old}) \cdot \left(\frac{R}{R + \exp(3.735 - 0.08835 \cdot h)} \right) \tag{16}$$

BD_{new}, BD_{old}	bulk density	[g cm^{-3}]
BD_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 (Equation 17).

$$R = P \cdot \left(\frac{1 + 2 \cdot \frac{S}{S + \exp(8.597 - 0.075 \cdot S)}}{(10 \cdot h)^{0.6}} \right) \tag{17}$$

R	factor of re-compaction	[-]
P	water percolation	[mm]
S	sand content	[%]
h	lower boundary layer	[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 (Equation 18).

$$BD = (2.631 + 15.811 \cdot b) \cdot \exp(b \cdot C_{org}) \tag{18}$$

The parameter b is determined site specifically during model initialisation. For a static calculation of bulk density Equation 24 can be used. Usually the observed BD is related to a specific sedimentation status of the soil. As a consequence, it is necessary to implement a re-compaction level (Equation 19).

$$BD_0 = BD(C_{org}) \cdot RC \tag{19}$$

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

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 (Equation 20 and Equation 21).

$$PV = \varepsilon_L + \varepsilon_W \cdot 1.09 \tag{20}$$

$$BD = (1 - PV) \cdot PD \tag{21}$$

PV	pore volume after thawing	[0..1]
BD	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 (Equation 22).

$$\Delta BD = f\_bioturb \cdot BAT \tag{22}$$

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

The parameter *f_bioturb* can be defined in the general parameters (CDYAPARM) – otherwise the standard value 0.001 is used.

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 is an appropriate alternative. This enables the estimation of required soil properties (e.g. field capacity, permanent wilting point) from other known and easily measureable properties (e.g. texture). Furthermore, the implementation of the dynamical description of soil structure in CANDY bases on the application of pedotransfer functions (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 (Equation 26) after Nemes et al. (1999) is useful.

$$STK = \frac{y_2 - y_1}{\log(x_2) - \log(x_1)} \cdot (\log(x) - \log(x_1)) + y_1 \tag{23}$$

STK	soil texture class	[M. %]
x	particle size diameter of the missing STK (upper limit)	[mm]
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 is described in chapter Soil structure dynamics (Equation 18). If only clay content and C_{org} content are available it is possible to calculate bulk density using Equation 24 (Ruehlmann and Körschens 2009).

$$TRD = 1.64 - 0.0075 \cdot T - 0.0611 \cdot C_{org} \tag{24}$$

Particle density

The particle density PD is calculated following an approach depending on actual C_{org} (Equation 23 to Equation 25) (Rühlmann et al. 2006).

$$PD = \left(\frac{Q_{os}}{\rho_{os}} + \frac{1 - Q_{os}}{\rho_{min}} \right)^{-1} \tag{25}$$

With:

$$\rho_{OS} = 1.127 + 0.373 \cdot Q_{OS} \tag{26}$$

$$Q_{OS} = \frac{C_{org}}{55} \tag{27}$$

Q_{OS}	volumetric part of organic matter	[-]
C_{org}	organic carbon content	[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 - initialisation phase)	[g cm^{-3}]

Pore Volume

The pore volume is based on the relation between bulk density and particle density.

$$PV = 1 - \frac{TRD}{TSD} \tag{28}$$

Water parameters according to Lieberoth

The simplest approach to calculate field capacity (Equation 27) and permanent wilting point (Equation 28) after Lieberoth (1982) is based on soil texture data only.

$$FC = 3.4 + 0.85 \cdot ABT \tag{29}$$

$$PWP = 1.23 + 0.74 \cdot T \tag{30}$$

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

$$\Theta(\Psi) = \Theta_r + \frac{\Theta_s - \Theta_r}{(1 + (\alpha \cdot |\Psi|)^n)^m} \tag{31}$$

α	van Genuchten parameter	[cm^{-1}]
n	van Genuchten parameter	[-]
m	van Genuchten parameter	[-]
Ψ	matric potential	[hPa]
Θ_r	residue water content	[0..1]
Θ_s	saturation water content	[0..1]

Approach of Vereecken

Vereecken et al. (1989) calculate the van Genuchten parameters using USDA7 texture classes (Equation 30 to Equation 34).

$$\Theta_s = 0.81 - 0.283 \cdot BD + 0.001 \cdot T \tag{32}$$

$$\Theta_r = 0.015 - 0.005 \cdot T + 0.014 \cdot C_{org} \tag{33}$$

$$\alpha = e^{(-2.486 + 0.025 \cdot S - 0.351 \cdot C_{org} - 2.617 \cdot BD - 0.023 \cdot T)} \tag{34}$$

$$n = e^{(0.053 - 0.009 \cdot S - 0.013 \cdot T + 0.00015 \cdot S^2)} \tag{35}$$

$$m = 1 \tag{36}$$

α	van Genuchten parameter	[cm⁻¹]
n	van Genuchten parameter	[-]
m	van Genuchten parameter	[-]
Ψ	matric potential	[hPa]
Θr	residue water content	[0..1]
Θs	saturation water content	[0..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 (Equation 35 to Equation 44).

For S < 66.5

$$\Theta_s = 0.788 - 0.263 \cdot BD + 0.001 \cdot T \tag{37}$$

$$\Theta_r = 0 \tag{38}$$

$$\alpha = e^{(-0.648 + 0.023 \cdot S - 3.1618 \cdot BD - 0.044 \cdot T)} \tag{39}$$

$$n = 1.392 + 1.212 \cdot T - 0.4189 \cdot S^{-0.024} \tag{40}$$

$$m = 1 - \frac{1}{n} \tag{41}$$

For S ≥ 66.5

$$\Theta_s = 0.89 - 0.322 \cdot BD + 0.001 \cdot T \tag{42}$$

$$\Theta_r = 0 \tag{43}$$

$$\alpha = e^{(-4.197 + 0.013 \cdot S - 0.276 \cdot BD - 0.076 \cdot T)} \tag{44}$$

$$n = -2.562 + 3.75 \cdot T^{-0.016} + 7 \cdot 10^{-9} \cdot S^{4.004} \tag{45}$$

$$m = 1 - \frac{1}{n} \tag{46}$$

α	van Genuchten parameter	[cm⁻¹]
n	van Genuchten parameter	[-]
m	van Genuchten parameter	[-]
Θr	residue water content	[0..1]
Θs	saturation water content	[0..1]

T	clay content	[M. %]
S	sand content	[M. %]
BD	bulk density	[g cm^{-3}]

Water retention model according to Brooks-Corey

$$\Theta(\Psi) = \begin{cases} \theta_r + (\theta_s - \theta_r) \cdot \left(\frac{\Psi}{\Psi_b}\right)^{-2} & ; \ \substack{\Psi > \Psi_b > \lambda > 0 \\ \Psi \leq \Psi_b} \\ \theta_S \end{cases} \tag{47}$$

$\Theta(\Psi)$	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) (Equation 46 to Equation 49) (Brooks 1964, Rawls and Brakensiek 1985).

$$\begin{aligned} \Psi_b = exp(&5.3396738 + 0.1845038 \cdot T - 2.48394546 \cdot PV - 0.00213853 \cdot T^2 - \\ &0.04356349 \cdot S \cdot PV - 0.61745089 \cdot T \cdot PV + 0.00143598 \cdot S^2 \cdot PV^2 - \\ &0.00855375 \cdot T^2 \cdot PV^2 - 0.00001282 \cdot S^2 \cdot T + 0.00895359 \cdot T^2 \cdot PV - \\ &0.00072472 \cdot S^2 \cdot PV + 0.0000054 \cdot T^2 \cdot S + 0.5002806 \cdot PV^2 \cdot T) \end{aligned} \tag{48}$$

$$\begin{aligned} \lambda = exp(&-07842831 + 0.0177544 \cdot S - 1.062498 \cdot PV - 0.00005304 \cdot S^2 - \\ &0.00273493 \cdot T^2 + 1.11134946 \cdot PV^2 - 0.03088295 \cdot S \cdot PV + 0.00026587 \cdot \\ &S^2 \cdot PV^2 - 0.00610522 \cdot T^2 \cdot PV^2) - 0.00000235 \cdot S^2 \cdot T + 0.00798746 \cdot T^2 \cdot PV - \\ &0.00674491 \cdot PV^2 \cdot T \end{aligned} \tag{49}$$

$$\theta_r = -0.0182482 + 0.00087269 \cdot S + 0.00513488 \cdot T + 0.02939286 \cdot PV - 0.00015395 \cdot T^2 - 0.0010827 \cdot S \cdot PV - 0.00018233 \cdot T^2 \cdot PV^2 + 0.00030703 \cdot T^2 \cdot PV - 0.0023584 \cdot PV^2 \cdot T \tag{50}$$

$$\theta_s = 0.01162 - 0.001473 \cdot S - 0.002236 \cdot T + 0.98402 \cdot PV + 0.0000987 \cdot T^2 + 0.003616 \cdot S \cdot PV - 0.010859 \cdot T \cdot PV - 0.000096 \cdot T^2 \cdot PV - 0.002437 \cdot PV^2 \cdot S + 0.0115395 \cdot PV^2 \cdot T \tag{51}$$

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]

Switching between the different pedotransfer functions for the hydrologic parameters can be done with the MS Windows Registry Editor choosing (see chapter Technical preparations):

ptfmode=1   for Rawls Brakensiek/Brooks-Corey

ptfmode=2   for Vereecken/van Genuchten

ptfmode=3   for Lieberoth

ptfmode=4   for Zacharias/van Genuchten

Biologic Active Time

Input

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

Output

symbol	description	unit	measurement id	result id
BAT	Biologic active time	[d]	52	104
mic_BAT	… in micropores	[d]	-	138
mes_BAT	… in mesopores	[d]	-	137
mac_BAT	… in macropores	[d]	-	136

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 a given time interval a certain biologic activity in a suboptimal environment will produce a specific turnover result. 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 taken into account. The annual BAT sum is an important indicator for the potential turnover under the given conditions.

The scheme in Figure 5 demonstrates the principle how different intensities of uniform time steps (Figure 5 A) are transformed into time steps of different length and uniform intensity (Figure 5 B). The calculated turnover, symbolized 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 5 B).

BAT is calculated in daily time steps for the 3 top soil layers (0-3 dm) and distributed to the pore space classes used in CIPS (chapter CIPS).
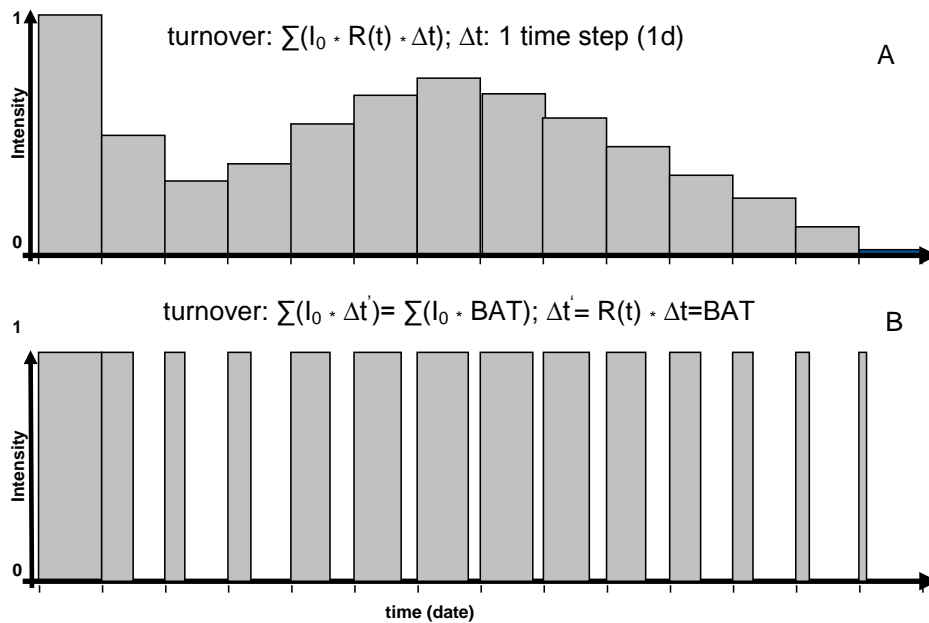
Figure 5: Schematic representation of the turnover calculation by the standard approach (A) and the BAT approach due to transformation of time steps (B).

Calculation of BAT is giving by Equation 50, as a function of time, including temperature (Equation 51), water (Equation 52) and aeration (Equation 53):

$$BAT = \Delta t \cdot R_T(T) \cdot R_\theta(\Theta) \cdot R_A(\varepsilon_L, h, FAT) \tag{52}$$

with:

$$R_T(T) = \min\left(Q_{10}^{(T-35)/10}\right); 1) \tag{53}$$

$$R_\theta(\Theta) = \min\left(4 \cdot \frac{\theta}{PV} * \left(1 - \frac{\theta}{PV}\right); 1\right) \tag{54}$$

$$R_A(\varepsilon_L, h, FAT) = \exp\left(-h \cdot \sqrt{\frac{\theta(FAT) \cdot R_T(T) \cdot R_\theta(\theta)}{\varepsilon_L \cdot (\varepsilon_L \cdot \varepsilon_P)}}\right) \tag{55}$$

R_x	reduction function of parameter x; $0 \leq R_x \leq 1$	[0..1]
Q_{10}	reaction quotient (Q_{10} = 2.1)	[-]
T	soil temperature	[°C]
PV	pore volume	[Vol. %]
Ɵ	soil moisture	[Vol. %]
h	depth	[dm]
FAT	clay and fine silt (particles ≤ 6.3 µm)	[M. %]
ε_P	relative pocket volume (const.)	[0..1]
ε_L	relative air volume	[0..1]
ϑ (FAT)	soil texture function (0.2844 · FAT - 1.4586; FAT ≥ 6)	[-]

Kommentar [EBb1]: Im paper steht cm. ???

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Soil organic matter turnover

Approach with conceptual pools

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	measurement id	result id
C_{org}	organic carbon content	[M. %]	7	-
C-SOM	amount of organic carbon in SOM (0-30cm)	[kg ha^{-1}]	28 [dt ha^{-1}]	91
C-AOM	amount of organic carbon in A-SOM (0-30cm)	[kg ha^{-1}]	-	90

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 pool	[d^{-1}]	CDYAPARM
k_S	rate coefficient for the C-flux from A-SOM to the S-SOM pool	[d^{-1}]	CDYAPARM
k_m	rate coefficient for the C-mineralization from the A-SOM pool	[d^{-1}]	CDYAPARM

Description

Soil organic matter (SOM) dynamics may be handled by different approaches. The original CANDY approach uses conceptual pools and describes C and N dynamics as well. The CIPS module uses measureable C pools and describes the long term stabilisation of SOM due to soil structure relations.

The SOM pools in the classical CANDY model have conceptual character and are not measurable (Figure 6).
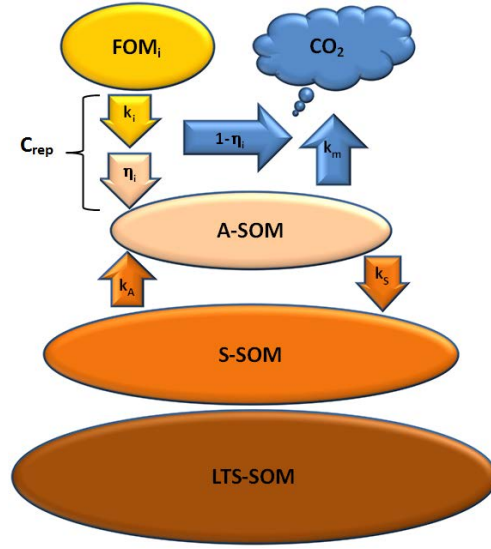
Figure 6: Conceptual pools and fluxes within the soil organic matter module in CANDY (description see text).

Soil organic matter is subdivided into four compartments: (1) fresh organic matter (FOM), (2) biological active soil organic matter (A-SOM or AOM), (3) stabilized soil organic matter (S-SOM or SSM) and (4) long term stabilized soil organic matter (LTS-SOM). 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}.

$$\frac{d\,C_{FOM}(t)}{dt} = k_{FOM}C_{FOM}(t) \tag{56}$$

$$\frac{d\,C_{REP}(t)}{dt} = \eta k_{FOM}C_{FOM}(t) \tag{57}$$

$$\frac{d\,C_{AOM}(t)}{dt} = \frac{d\,C_{REP}(t)}{dt} - (k_m + k_s)C_{AOM}(t) + k_a C_{SOM}(t) \tag{58}$$

$$\frac{d\,C_{SOM}(t)}{dt} = k_s C_{AOM}(t) - k_a C_{SOM}(t) \tag{59}$$

C_x	carbon content of corresponding compartments of SOM	[kg C ha^{-1}]
k	rate coefficient	[d^{-1}]
η	dimensionless synthesis coefficient	[-]

For the initialization of the CANDY model, the C amount of the LTS-SOM pool must be calculated. It is possible to choose from three different calculation methods: Fine particles after Körschens (Equation 58), clay content after Rühlmann (1999) (Equation 59) and particle surface after Puhlmann (Equation 60) and after Kuka (Equation 61) (Korschens 1980, Kuka 2005, Puhlmann et al. 2006).

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$$C_{LTS} = ICP \cdot FAT \tag{60}$$

$$C_{LTS} = 1.097 \cdot \left(1 - exp(-0.0747 \cdot T)\right) \tag{61}$$

$$C_{LTS} = C_{MIP} \tag{62}$$

with:

$$C_{MIP} = C_{org} \frac{A_{micro}}{A_{micro} + A_{meso} + A_{macro}} \tag{63}$$

$$A_m = 2 \frac{V_m}{R_m}, m \in \{micro, meso, macro\} \tag{64}$$

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. %]
ICP	parameter (~ 0.05)	[-]
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 ·10^{-7}, 10 ·10^{-7} and 500 ·10^{-7} for micro, meso and macropores, respectively)	[m]

Carbon In Pore Space (CIPS) approach

Input

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

Output

Symbol	description	unit	measurement_id	result_id
C{pool}{pore}	total C amount of a given pool (DOM, ROM, AOM)	[kg ha^{-1}]	-	Total: 991,992,993 (0-3 dm)
Age	age of the different C pools in a pore space (micro, meso, macro)	[y]	-	
	AOM			904,905,903
	ROM			902,900,909
	-or the average pool age			
	FOM, ROM, AOM			906,907,908
C_{org}	organic carbon content	[M. %]	7	

Parameters

Symbols	description	unit	source/value
α_{AOM}	partitioning coefficient for the AOM pool	[-]	0.30
η_{DOM}	efficiency coefficient for the DOM pool (DOM→AOM)	[-]	0.77
η_{ROM}	efficiency coefficient for the ROM pool (ROM→AOM)	[-]	0.65
η_L	efficiency coefficient (FOM→AOM) for the FOM_L pool from crop residues (eta_l_cr) or manure (eta_l_om)	[-]	crop residues: 0.5 org. manure : 0.4 or via CDYAPARM
η_R	efficiency coefficient (FOM→AOM) for the FOM_R pool from crop residues (eta_r_cr) or manure (eta_r_om)	[-]	crop residues: 0.7 org. manure: 0.55 or via CDYAPARM
k_{AOM}	rate coefficient for the decomposition of A-SOM pool	[d^{-1}]	0.055
k_{DOM}	rate coefficient for the decomposition of the DOM pool	[d^{-1}]	0.429

k_{ROM}	rate coefficient for the decomposition of the ROM pool	$[d^{-1}]$	0.0011
k_L	rate coefficient for the decomposition of the FOM_L pool	$[d^{-1}]$	0.25
k_R	rate coefficient for the decomposition of the FOM_R pool	$[d^{-1}]$	0.008

Description

The CIPS model did overcome the necessity of empirical (conceptual) pools by taking into account soil structure effects and measurable pools (Figure 7 and Figure 8).

Following the usual convention that SOM is represented by the amount of organic carbon, and leaving the fresh organic matter (FOM) fraction as an external pool, the total amount of organic carbon (Corg) is represented by the sum of all soil borne carbon pools (Equation 63). Active organic matter (AOM) is the microbial biomass that is determined using the substrate induced respiration (SIR) method. Dissolved organic matter (DOM) can be measured by common methods, but is usually neglected during model initialisation.

$$C_{org} = AOM + ROM + DOM \tag{65}$$

The general approach is characterized by:

- the division of SOM in qualitative pools on the basis of chemical measurability
- the dependence of the turnover conditions in terms of BAT (see chapter Biologic Active Time) from the location of SOM in pore space
- the structure dependent accessibility for microbial biomass

The organic material enters the soil via the pool of fresh organic matter (FOM). The FOM pool is fed by plant residues and organic manure. According to its solubility in water and microbial degradability the FOM material is divided into:

- the soluble fraction (FOM_S)
- the insoluble part is separated according to its resistance against microbial attacks in
  - labile (FOM_L)
  - resistant (FOM_R)

The active organic matter (AOM) is considered as an equivalent to microbial biomass. It is the only living component acting as an engine of carbon turnover in soil.

Dissolved organic matter (DOM) is produced during the decay of other pools or may be imported with the soluble part of FOM.

Refractory organic matter (ROM) represents the insoluble product of microbial decay. This pool is considered as very resistant against microbial decomposition. Finally, all decay processes feed the pool of carbon dioxide (CO_2).
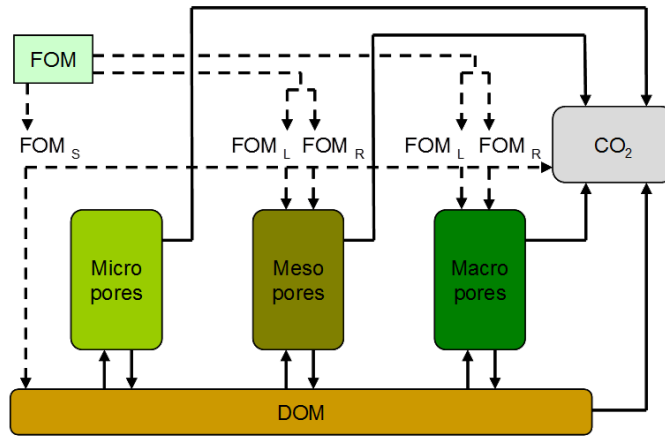
FOM   Fresh Organic Matter   DOM   Dissolved Organic Matter
   FOM_S Soluble fraction of FOM CO_2 Carbon dioxide
   FOM_L Labile fraction of FOM   - - →   Input in pore spaces
   FOM_R Resistant fraction of FOM   ⟶   Fluxes between pore classes

Figure 7: Exchange of carbon in pore space classes (Kuka et al (2007)
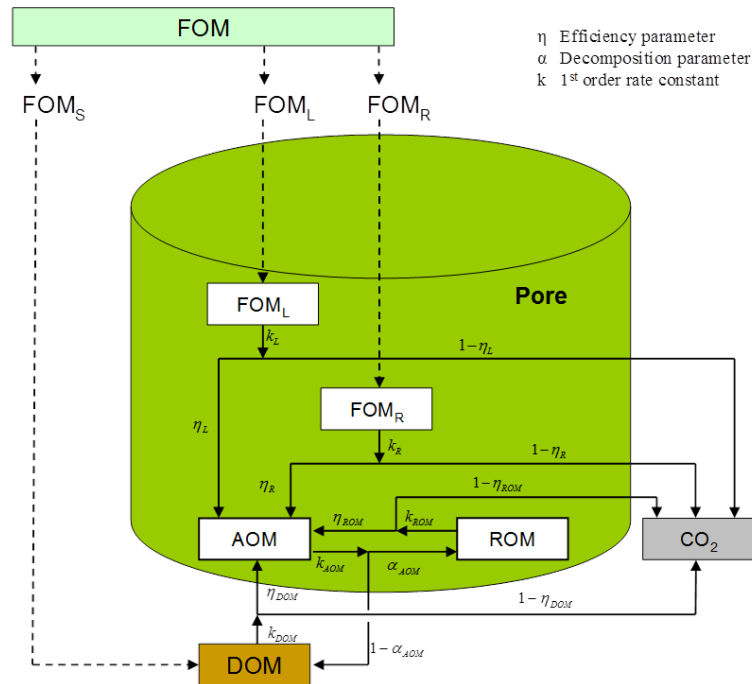
η   Efficiency parameter
α   Decomposition parameter
k   1st order rate constant

FOM   Fresh Organic Matter   AOM   Active Organic Matter
   FOM_S Soluble fraction of FOM   ROM   Refractory Organic Matter
   FOM_L Labile fraction of FOM CO_2 Carbon dioxide
   FOM_R Resistant fraction of FOM   - - →   Input in pore spaces
DOM   Dissolved Organic Matter   ⟶   Fluxes between pools

Figure 8: Pools and fluxes of the CIPS-model (Kuka et al (2007)

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As shown in Figure 7 the pools are assigned to different pore space classes. According to their equivalent radius, soil pores are divided into three classes: micro-, meso- and macropores. The micropores represent the pore space of the permanent wilting point and the mesopores the pore space of available field capacity. The macropores correspond to the remaining pore space. The FOM_L and FOM_R are only available for the AOM in meso- or macropores, because it is assumed that micropores are too small for organic matter particles. The FOM_S directly feeds the DOM pool, which itself is available to all pore space classes providing a vehicle for matter exchange between them.

In every pore space class, equal pools are characterized with an identical set of parameters. Figure 8 shows the carbon fluxes between the carbon pools in each pore space class. With the decomposition of the FOM_L, FOM_R, DOM and ROM pool carbon dioxide is produced and the biomass pool grows. The biomass pool itself decomposes into ROM and DOM. Equation 66 to Equation 69 describe the turnover dynamics for each pore space class with first-order kinetics and are based on the Biologic Active Time (BAT).

The total BAT of one time step is distributed to the single pore space classes according to their water saturation status (Kuka et al. 2007). If the soil water content is above field capacity it is assumed that all biological activity is located at the macropores. With reducing soil moisture, the biological activity is shared between two pore space classes. BAT is split between macro- and mesopore space if soil moisture is above the wilting point, and between meso- and micropore space if the soil moisture is further reduced below the wilting point. This principle follows the hypothesis, that biological activity needs free aeration as well as wetted surfaces. If one pore space class is completely drained, the biological activity in this class (BAT_{larger}) is controlled by the part of surface that is still wet (Equation 64). This is represented by the volumetric water content of the next smaller pore space class ($BAT_{smaller}$) (Equation 65).

$$BAT_{larger} = \frac{V_W}{V_W + V_A} \cdot BAT_{tot} \tag{66}$$

$$BAT_{smaller} = \frac{V_A}{V_W + V_A} \cdot BAT_{tot} \tag{67}$$

BAT_{larger}	see text above	[d]
$BAT_{smaller}$	see text above	[d]
V_W	water saturated volume of the smaller pore space class	[Vol. %]
V_A	air filled volume of the smaller pore space class	[Vol. %]
BAT_{tot}	total Biologic Active Time	[d]

As indicators for chemical pool stability, the *k*-values describe the matter breakdown. The efficiency parameters (η), as well as the decomposition parameter (α_{AOM}) are used to split the matter flux between two destinations.

The AOM pool representing the microbial biomass is fed by the decomposition of the labile and resistant fraction of FOM (η_L, η_R) and by the inputs from ROM and DOM decay (Equation 66). The autolytic AOM decay (k_{AOM}) is distributed into ROM (α_{AOM} in Equation 67) and DOM (1- α_{AOM} in Equation 68).

$$\frac{dAOM}{dt} = k_L\eta_L FOM_L + k_R\eta_R FOM_R + k_{ROM}\eta_{ROM}ROM + k_{DOM}\eta_{DOM}DOM - k_{AOM}AOM \quad (68)$$

The ROM pool is building up with products of the AOM pool decay (Equation 67). It decomposes itself and the matter flux is split into AOM (η_{ROM} in Equation 66) and CO_2 ($1-\eta_{ROM}$ in Equation 69).

$$\frac{dROM}{dt} = k_{AOM}\alpha_{AOM}AOM - k_{ROM}ROM \quad (69)$$

The DOM pool has an important function for the exchange of carbon between the different pore space classes. The AOM in all pore space classes may grow on this carbon source and during its decay it is feeding this pool as well (Equation 68).

$$\frac{dDOM}{dt} = FOM_S + k_{AOm}(1 - \alpha_{AOM})AOM - k_{DOM}DOM \quad (70)$$

The first term of Equation 68 represents the direct input from the soluble fraction of FOM into the DOM pool. Further matter input results from the decomposition of AOM. The DOM is consumed by microbial biomass resulting in a growth of the AOM pool (η_{DOM} in Equation 66) with a partial decomposition to CO_2 ($1-\eta_{DOM}$ in Equation 69).

Equation 69 shows the sum of all mineralization fluxes into CO_2 appearing during the growth of AOM.

$$\frac{dCO_2}{dt} = k_{DOM}(1 - \eta_{DOM})DOM + k_{ROM}(1 - \eta_{ROM})ROM + k_L(1 - FOM_L)FOM_L + \\ k_R(1 - \eta_R)FOM_R \quad (71)$$

Beside the basic pool dimensions the CIPS model also calculates the age (A) or the duration of the stay of carbon in these pools. The actual age of a pool is calculated in every time step as weighed means by pool contents (C), exports (E) and imports (I).

$$A_i^{new} = 1 + \frac{A_i^{old}\cdot\left(C_i^{old} - E_i\right) + \sum A_j \cdot I_j}{C_i^{old} - E_i + \sum E_j} \quad (72)$$

To all external influxes (fertilization and plant residues) an age of zero is assigned. The initial age of all pools is read from the file cips_i.ini in the CANDY data dictionary. The file contains the initial values of the pool size (SIZE) as well as the pool age (AGE) of ROM, AOM and DOM.

If the model options include soil structure dynamics the results of that module are used for a re-distribution of the carbon on the pore classes. Depending on the structural changes the organic matter on the pore surface is transferred into a bigger (loosening) or smaller (compaction) pore class (Equation 71 and Equation 72).

$$\Delta A_{mic} = \begin{cases} \dfrac{PWP_{old} - PWP_{new}}{PWP_{old}} & \text{if } PWP_{old} > PWP_{new} \\[2ex] \dfrac{PWP_{old} - PWP_{new}}{FK_{old} - FK_{new}} & \text{if } PWP_{old} < PWP_{new} \end{cases} \tag{73}$$

$$\Delta A_{mes} = \begin{cases} \dfrac{FK_{old} - FK_{new}}{FK_{old} - PWP_{old}} & \text{if } FK_{old} > FK_{new} \\[2ex] \dfrac{FK_{old} - FK_{new}}{PV_{old} - FK_{old}} & \text{if } FK_{old} < FK_{new} \end{cases} \tag{74}$$

An alteration of the C pools arises from the changes of the surfaces in another pore class (Equation 73 to Equation 75).

$$\Delta C_{mic} = \begin{cases} -\Delta A_{mic} \cdot C_{mic} & \text{if } \Delta A_{mic} > 0 \\[1ex] -\Delta A_{mic} \cdot C_{mes} & \text{if } \Delta A_{mic} < 0 \end{cases} \tag{75}$$

$$\Delta C_{mes} = \begin{cases} \Delta A_{mic} \cdot C_{mic} & \text{if } \Delta A_{mic} > 0 \\[1ex] \Delta A_{mic} \cdot C_{mes} & \text{if } \Delta A_{mic} < 0 \\[1ex] -\Delta A_{mes} \cdot C_{mes} & \text{if } \Delta A_{mes} > 0 \\[1ex] -\Delta A_{mes} \cdot C_{mac} & \text{if } \Delta A_{mes} < 0 \end{cases} \tag{76}$$

$$\Delta C_{mac} = \begin{cases} -\Delta A_{mes} \cdot C_{mes} & \text{if } \Delta A_{mes} > 0 \\[1ex] -\Delta A_{mes} \cdot C_{mac} & \text{if } \Delta A_{mes} < 0 \end{cases} \tag{77}$$

All pool sizes are calculated with Equation 76:

$$C_{new} = C_{new} + \Delta C \tag{78}$$

N dynamics

Input

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

Output

symbol	description	unit	measurement_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 mineralization	N_{min} transfer from/to SOM (mineralization: "+", immobilization: "-")	[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 volatilization	[kg ha^{-1}]	-	123
N$_2$O emission	N$_2$O-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 parameterset	decision support system for nitrogen fertilization (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 9).
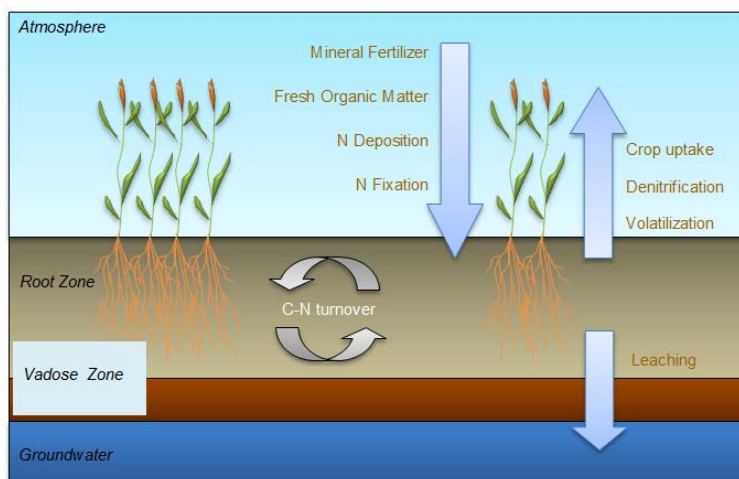

Figure 9: Schematic representation of N dynamics in the CANDY model

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

Sources

- N deposition
- Input from land management
  - Mineral fertilizer
    - application of fertilizer
    - autofertilization (goal oriented or SBA method)
  - Fresh organic matter
    - organic amendments
    - crop residues
- C-N turnover
  - N mineralization (ammonification)
  - nitrification
  - N immobilization
- N fixation by legumes

Sinks

- plant uptake
- N exports to environment
  - N leaching
  - gaseous losses (denitrification, volatilization)

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)   → standard: 0.17

     N_IM_SOM (immission for summer season)   → standard: 0.71

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 fertilizer 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 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.

Autofertilization

SBA method (german: Stickstoff-Bedarfs-Analyse)

For scenario simulations there is often no information available about the actual fertilization rates. In order 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, since N may be split between these two dates in case of high doses. 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.

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. If not enough mineral nitrogen is available, the decomposition rate is reduced in order to avoid negative N_{min}.

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 top soil.

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 according to Equation 77.

$$N_L = N_{NO_3} \cdot \left(1 - D \cdot \frac{PWP}{FC}\right) \cdot \frac{P}{\Theta_0} \tag{79}$$

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 volatized.

Gaseous losses from nitrate N are calculated as a result of anaerobic turnover. Whereas 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 (Equation 78):

$$R_\Theta = \sqrt{\frac{\Theta + 0.627 \cdot FC - 0.0267 \cdot PV \cdot FC}{1.627 \cdot FC - 0.0267 \cdot PV \cdot FC}} \tag{80}$$

R_Θ	reduction function for soil moisture impact on denitrification	[-]
FC	water content at field capacity	[Vol. %]
PV	soil pore volume	[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.

$$N_{deni} = MIN\left(MAXDENI, k_{deni} \cdot R_\Theta \cdot R_T \cdot N_{NO_3} \cdot C_{AOM}\right) \tag{81}$$

N_{deni}	denitrificated 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 (Equation 80 to Equation 83) (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}).

$$f_{wfps} = \frac{1.4}{13^{\left(\frac{17}{13^{(2.2 \cdot wfps)}}\right)}} \tag{82}$$

with

$$wfps = \frac{\theta}{PV} \tag{83}$$

$$f_{CO_2} = 13 + \frac{30.78 \cdot \arctan\left(\pi \cdot 0.07 \cdot (P_{CO_2} - 13)\right)}{\pi} \tag{84}$$

$$f_{NO_3} = 25 \cdot \left(1 - \left(0.5 + \frac{\arctan\left(\pi \cdot 0.01 \cdot (C_{NO_3} - 190)\right)}{\pi}\right)\right) \tag{85}$$

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 (Equation 84).

$$R_{N_2/N_2O} = f_{wfps} \cdot \sqrt{\left(f_{NO_3} \cdot f_{CO_2}\right)} \tag{86}$$

Finally the resulting N_2O flux (N_{N2O}) is calculated with Equation 85.

$$N_{N_2O} = \frac{N_{deni}}{1 + R_{N_2/N_2O}} \tag{87}$$

Crop module

Crop development

The selection of plant modules in CANDY is enabled by the hierarchical principle in the model structure. I.e. the crop dynamics is already represented by four crop variables (crop height, root depth, coverage, N uptake) independent of the internal complexity of the selected plant module.

The plant modules, CANDY_S and GRASSLAND, will be described in the following.

CANDY_S approach

Input

symbol	description	unit	source
WERT1	Crop ID	[-]	CDY_MADAT
DATUM	date of sowing	[-]	CDY_MADAT (MACODE = 12)
DATUM	date of emergence	[-]	CDY_MADAT (MACODE = 1)
DATUM	date of harvest	[-]	CDY_MADAT (MACODE = 2; 9)
WERT2	Yield of main product	[dt ha^{-1}]	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) 56 (per layer)	202 (sum) 122 (flux)
BG	cover grade	[0..1]	46	127
T	current root depth	[dm]	45	-

Parameters

symbol	description	unit	source
ITEM_IX	Crop ID	[-]	CDYPFLAN
NAME_engl	crop name in English	[-]	CDYPFLAN
NAME	crop name in German	[-]	CDYPFLAN
NAME_lat	crop name in Latin	[-]	CDYPFLAN
ART	1 = summer crop	[-]	CDYPFLAN
	2 = winter crop		
	3 = annual legume crop		
	4 = perennial legume crop		
	5 = perennial crop		

MODELL	model algorithm, CANDY_S or CDYDGRN	[-]	CDYPFLAN
TRANSK	transpiration coefficient (only used with switch V+ in CANDY_S)	[-]	CDYPFLAN
ALGO	characteristic of plant (annual or perennial crop)	[-]	CDYPFLAN
STEIL (S)	slope parameter for S curve (N uptake)	[-]	CDYPFLAN
VEGDAU (V)	days from emergence to harvest	[d]	CDYPFLAN
NBOK	N_{min} uptake rate of legumes from soil	[0..1]	CDYPFLAN
LNUB	part of N stored in subsoil	[0..1]	CDYPFLAN
WTMAX	maximum root depth	[dm]	CDYPFLAN
WWG	days for 10 cm root depth growth	[d]	CDYPFLAN
DBHMAX	days from emergence to maximum crop height	[d]	CDYPFLAN
BHMAX	maximum crop height	[cm]	CDYPFLAN
MATANF	days from starting maturity to ripeness	[d]	CDYPFLAN
TEMPANF	days from emergence to beginning influence on soil temperature	[d]	CDYPFLAN
BGMAX	maximum crop coverage	[0..1]	CDYPFLAN
DBGMAX	days from emergence to maximum crop coverage	[d]	CDYPFLAN
CEWR	N amount in harvest residues independent from yield	[kg ha^{-1}]	CDYPFLAN
FEWR	factor between N in harvest residues + roots and N yield	[-]	CDYPFLAN
N_GEHALT	N content in aboveground biomass (yield + by-product)	[%]	CDYPFLAN
Czep	specific interception capacity related to plant height	[mm cm^{-1}]	CDYPFLAN
Zetb	parameter of water withdrawal function	[-]	CDYPFLAN
EWR_IX	pointer to a record in CDYOPSPA to characterise harvest residues and roots	[-]	CDYPFLAN
GRD_IX	pointer to a record in CDYOPSPA to characterise aboveground biomass after ploughing up	[-]	CDYPFLAN
SBA_ID	pointer to a record in SBACROP to characterise crop	[-]	CDYPFLAN

	for automatic fertilization		
HI	relation of by-product to main product	[-]	CDYPFLAN
KOP_IX	pointer to a record in CDYOPSPA to characterise by-product	[-]	CDYPFLAN

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 10).
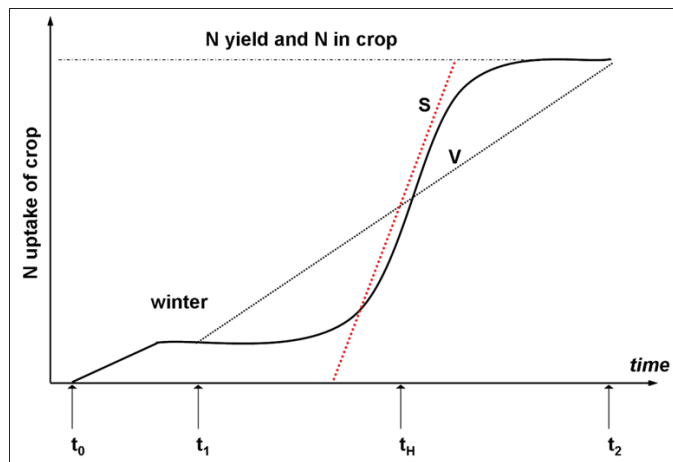

Figure 10: Definition of the N uptake at crop emergence (t_0), start (t_1) and end (t_2) of the vegetation period (V = crop parameter VEGDAU) in the harvest year and the inflexion point ($t_H = (t_2 - t_1)*0.5$).
(S = crop parameter STEIL)

The mathematical formulation is given by Equation 86 (Franko et al. 1995):

$$N_{upt}(t) = 0.5 \cdot \left(1 + \frac{\tan\left(\frac{2t}{V-1}\right) \cdot S}{\tan(S)}\right) \cdot N_{total} \tag{88}$$

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 if plant roots are apparent in a calculation layer. The rooting depth is calculated by an interpolation of WTMAX (crop specific maximum rooting depth) and WWG (days for 10 cm root depth growth). The development of rooting depth is a steady process until it reaches the maximum. Afterwards the rooting depth remains constant until the harvest. If the

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 harvest residues and roots (Equation 87).

$$N_{res} = \frac{N_{upt} \cdot FEWR \cdot CEWR}{1 + FWER} = CEWR + N_{yield} \cdot FEWR \qquad (89)$$

N_{res}	N amount from harvest residues and roots	[kg N ha^{-1}]
N_{upt}	total N in crop (yield + by-product + roots and residues)	[kg N ha^{-1}]
N_{yield}	N amount in main and by-product	[kg N ha^{-1}]
CEWR	N amount in harvest residues independent from yield	[kg N ha^{-1}]
FEWR	factor between N in harvest residues and roots and N yield	[-]

The plant development parameters (plant height BH and coverage BG) are calculated as interpolation of days from emergence to time of maximum development (DBHMAX and DBGMAX) and their maximum values (BHMAX and BGMAX) (Figure 11). Additionally, the coverage is influenced by the senescence of the crop. Plant development is considered as independent from nitrogen uptake. The parameter MATANF 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. However, some crops have a slow development in the youth stage. TEMPANF is the parameter that regulates the beginning of the effect on soil temperature.

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.
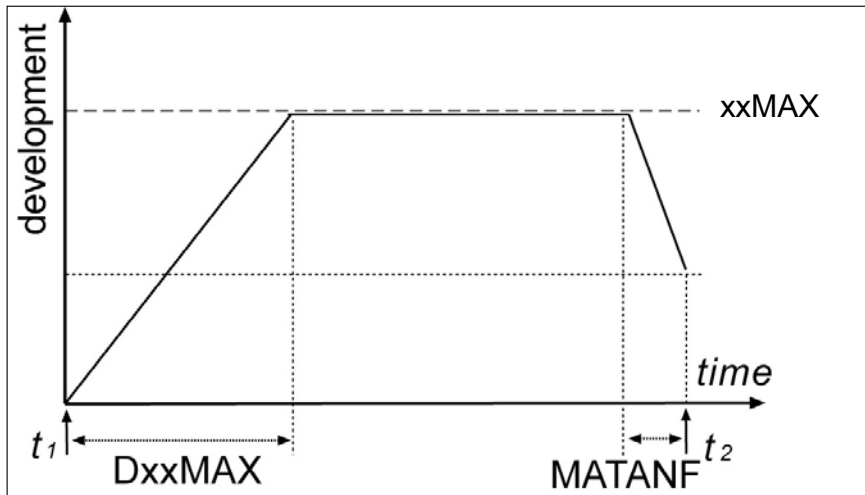

Figure 11: Development of rooting depth, crop height and coverage with xxMAX: WTMAX (maximum rooting depth), BHMAX (maximum plant height), BGMAX (maximum plan coverage) and MATANF (days of senescence) as plant parameters within the table CNDPFLAN as interpolation of days between start (t₁) and end (t₂) of the vegetation period.

Legumes

Input

See crop module

Output

See crop module

Parameter

See crop module

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 ART defines a plant type (ART=3: annual legume crop, ART=4: perennial legume crop). Additional to the organic bound N amount of the residues, CANDY considers a certain amount of inorganic N that is equally deposited in the subsoil (Equation 88).

$$N_{res} = N_{res} \cdot (1 - LNUB) \tag{90}$$

LNUB   part of N stored in subsoil   [0..1]

The fixation of atmospheric nitrogen is given by Equation 89 and Equation 90.

$$N_{sym} = N_{dem} \cdot (1 - NBOK) \tag{91}$$

$$N_{soil\_up} = N_{dem} - N_{sym} \tag{92}$$

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}]
NBOK	part of N uptake from soil N_{min} pool	[0..1]

Permanent Grasslands

Input

symbol	description	unit	source
LTEM	daily air temperature	[°C]	CDY_CLDAT
ET_a	actual evapotranspiration	[mm]	internal
iLCU	increase of livestock units		CDYMADAT (MACODE = 10)
dLCU	decrease of livestock units		CDYMADAT (MACODE = 11)

Output

See crop module

Parameters

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

Description

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 N uptake of the crop is controlled by the temperature sum and the actual evapotranspiration. If air temperature is above 4°C the daily N uptake is calculated by Equation 91 to Equation 95.

$$TS = TS + LTEM - 4 \tag{93}$$

$$TRANSKO = TK_{max}; TS \leq TS_1 \tag{94}$$

$$TRANSKO = TK_{min} + (TK_{max} - TK_{min} \cdot N) \cdot \frac{TS_2 - TS}{TS_2 - TS_1}; \ TS_1 < TS < TS_2 \tag{95}$$

$$TRANSKO = TK_{min}; TS \geq TS_2 \tag{96}$$

$$N_{up} = N_{up} + TRANSKO \cdot ET_a \tag{97}$$

TS	temperature sum	[-]
LTEM	daily air temperature	[°C]
TRANSKO	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}]
ET_a	actual evapotranspiration	[mm]

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 (Equation 96 and Equation 97). Animal faeces are treated as organic amendments (Equation 98). 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.

$$N_{AU} = N_{AU} + \Delta N_{AU} \tag{98}$$

$$N_{GR} = N_{AU} + N\_UPT \tag{99}$$

$$C_{OA} = N_{AU} + N\_INP \tag{100}$$

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}]

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