CCB Manual

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1 Introduction

1.1 Development of CCB (purpose)

CCB (CANDY carbon balance) is a simplified version of the carbon dynamic model in CANDY (find the CANDY manual under www.ufz.de/candy). It describes the turnover of decomposable carbon in annual time steps for average site conditions depending on crop yields, input rates of fresh organic matter and the initial organic carbon content of the soil. The biologic active time is estimated from site conditions (soil physical parameters of the top soil, tillage system, average rainfall and air temperature) if not known from CANDY simulations. Outputs of CCB include dynamics of total organic carbon, SOM reproduction and Nitrogen mineralization.

The model has been validated using a dataset from 40 long-term experiments situated in Central Europe including 391 treatments with a total number of 4794 C_{org} observations. Statistical measures to prove model validity were mean error (ME = -0.001) and root mean square error (RMSE = 0.119). In addition a number of tests were performed to make sure that the model has no systematic error for different types of site conditions and management activities.
After this successful validation the CCB model is considered applicable for advisory service for arable fields on a wide range of site conditions.

1.2 Overview of CCB

The CCB model can be used in different workflows depending on the modelling demands, data availability and scale of interest. The standard workflow is considering the simulation on field scale including the availability of C_{org} measurements for the parameterization of the initial concentration and the validation of the simulation.
Key procedures of the standard workflow are:

- Simulation of soil carbon concentration, soil carbon mineralization, soil carbon reproduction on annually time step
- Simulation of soil nitrogen dynamics (esp. N-mineralization from fresh organic matter and soil organic matter) on annually time step
- Within the model setup it is possible to consider the following criteria:
    - crop rotations, crop yield, handling of by-products,
    - application of organic manure and mineral fertilizer
    - soil properties of the topsoil (e.g. soil texture)
    - climate data (temperature, rainfall)
    - conventional tillage and reduced tillage (conservation tillage)
    - irrigation

Furthermore the CCB model system can be used in several “expert” modes which adapt CCB to special modelling demands that mainly result from special situations of data availability. These special application cases are described in section 2.6 and cover the topics:

- Indicator based simulation: Assessment of the humus supply level without the need of measurement data for C_{org}.
- Simulation of a pre-treatment: If an experiments starts with considerable changes of the management it may be reasonable to include the history of this place in the simulations.
- Simulation in ‘regional-mode’: Developed for meso to large scale studies. Inter alia crop share statistics can be used as data input instead of crop rotations.

The following chapters contain an user guide for the program interface and then provide a more detailed description of the algorithms implemented in CCB together with an explanation of the model parameters (‘3 Theoretical Documentation’). The description of the program interface is based on the standard workflow. Information concerning the expert mode are only mentioned where necessary and are described in an extra section at the end of the Theoretical Documentation. Finally section ‘4 Input-/Output Parameters & Database’ describes the CCB Database and its manipulation.

2 Interface of CCB

2.1 Install Interface / Initialization

To start the CCB model following files are necessary:

- CCB Exe file (e.g. CCB_2016.exe)
- borlndmm.dll (library necessary to run CCB)
- CCB compatible database (e.g. CCB_sample_db.mdb)

The best way for a first start is to copy all files in one directory. Then start the CCB exe file and the program is asking for a connection to a CCB compatible database (when starting CC the very first time):

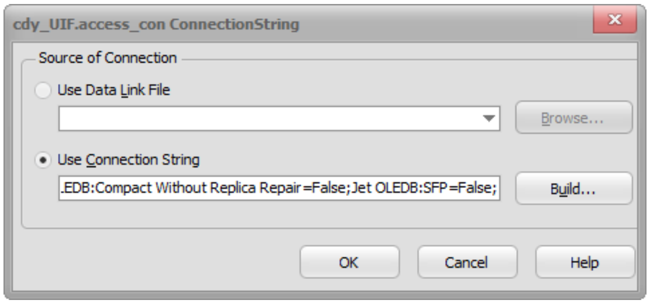


Figure 1: Start the creation of a CCB database connection

Click on [Build] to tell the model how it can connect to the database file.

First step is the specification of a DB-Provider. The selection of "*Microsoft Jet 4.0 OLE DB Provider*" is recommended, but "*Microsoft Office 12.0 Access Database Engine OLE DB Provider*" works as well.

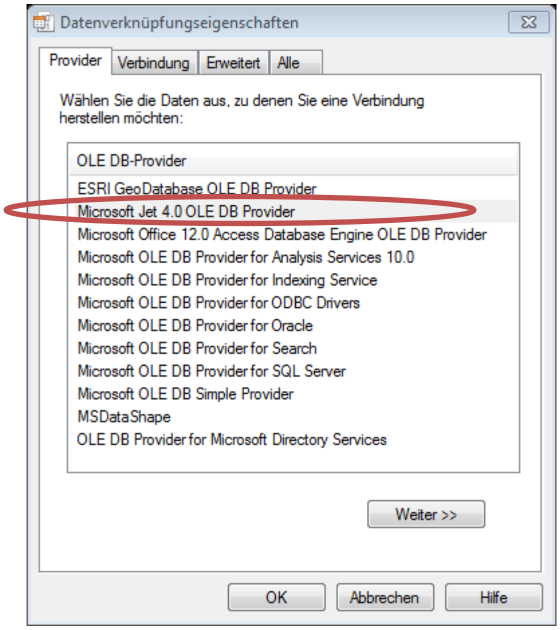


Figure 2: Selection of database provider

Select the provider and click [Weiter]. Then you have to specify the filename (and path) of the CCB – Access-Database that you have got together with CCB.exe. It is strongly recommended to make a copy of the template and give it a name that reminds you to the content (like ccb_my_experiment.mdb)

In the next step you have to select this file. This is easy with the Jet 4 Provider. Just click on […] and open the file.

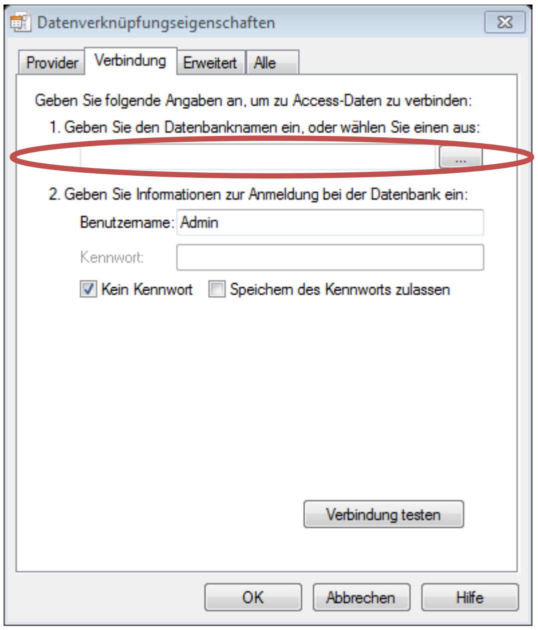


Figure 3: Selection of the CCB database

After finishing this step click on [Ok] (you may check the connection with [Verbindung testen] but if you don’t mix up the file names it should work anyway.

Now you see:

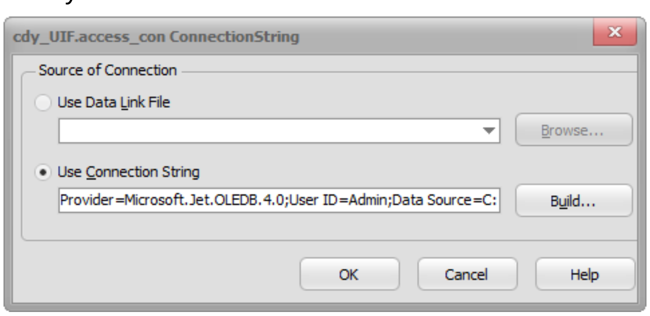


Figure 4: Finish the creation of a CCB database connection

Click [Ok] and you should have a proper running CCB program showing its data connection in a listbox.

CCB will store the information about this data connection in the registry of the computer system and on the next start it will try to connect to the same database. If this fails you will be asked to select the desired file.

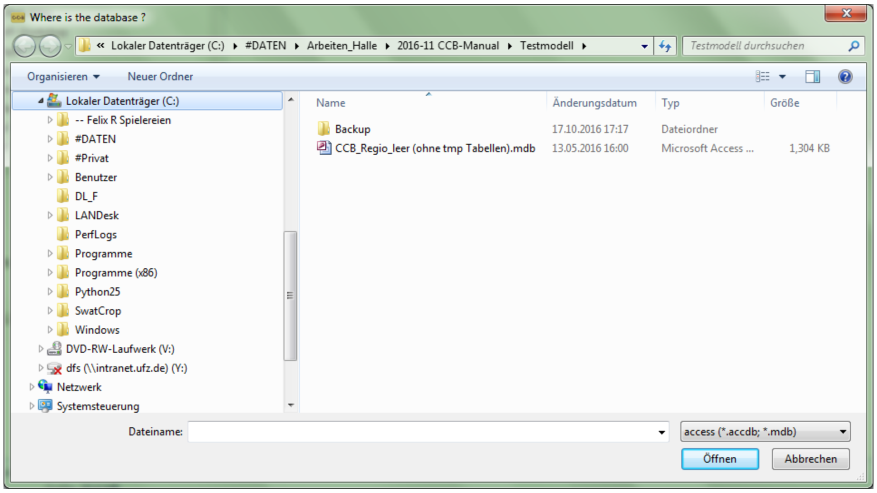


Figure 5: Selection of CCB database when connection fails.

2.2 Main Interface

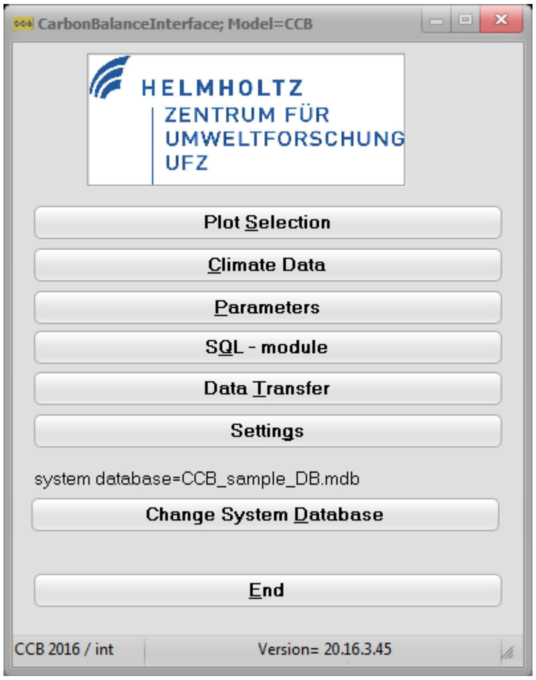


Figure 6: CCB main interface

This main form provides following menu items:

Plot Selection: data input , model start and result presentation

Climate Data: Edit climate data (weather and N-deposition)

Parameters: View and edit model parameters

SQL – module: Tool to run short sql scripts

Data Transfer: Move selected data sets into another database

Settings: Check and change the configuration n

Change System Database: Select the database

2.3 Data input

2.3.1 Generation of experiments & plots

First step is the selection of the database containing model parameters and user specific data. The last used database is shown at the lower part above the button „*Change System Database“.* If this field is empty or if the database shall be changed – click on the button and select the appropriate file from the standard windows dialog.

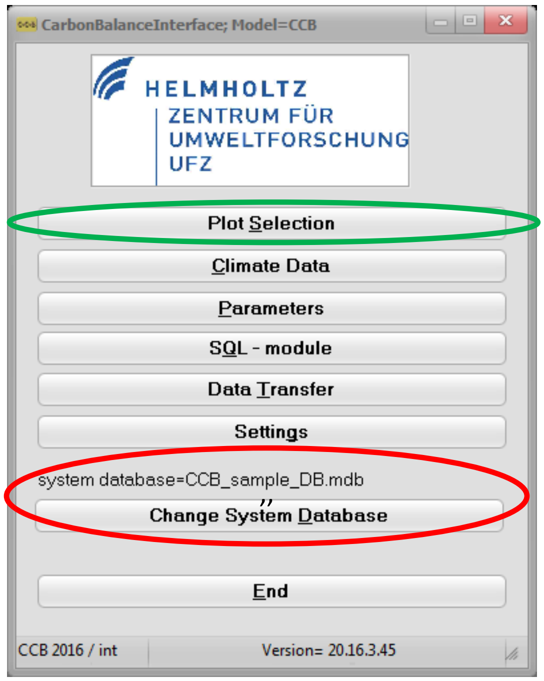


Figure 7: Database selection (red circle) and editing user data (green circle)

The data in CCB are usually organised as treatments (*plots*) of an *experiment*. Each experiment may contain numerous plots and one database can contain several experiments. Of course an experiment has not to be a real one – it may contain as well records of different farm fields or similar units. Click on "Plot Selection to start editing your data.

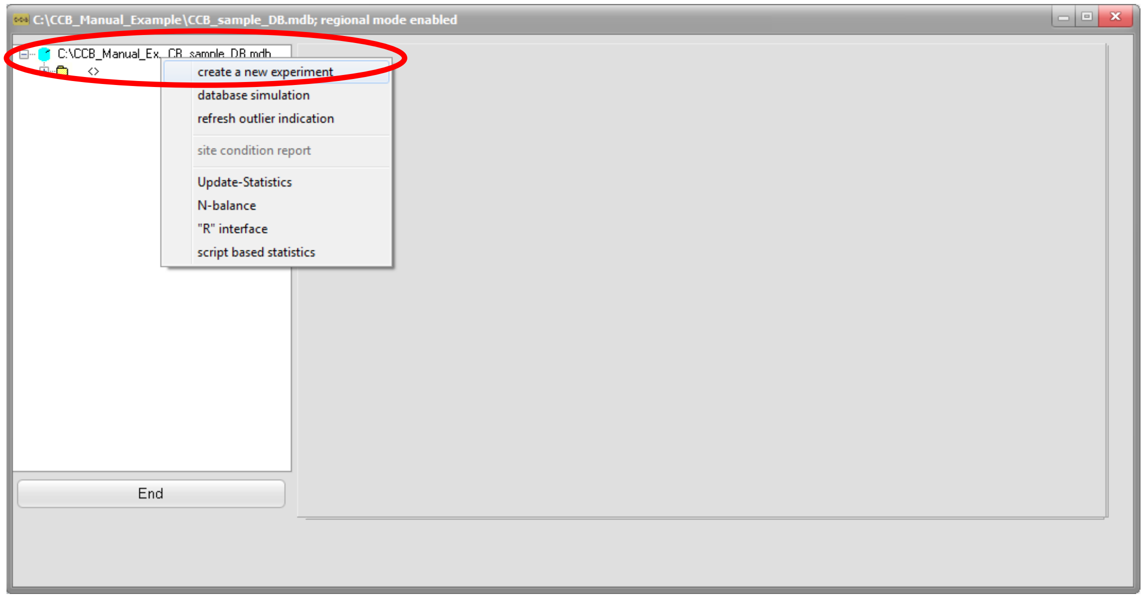


Figure 8: Create a new experiment folder

A right click on the path of your current database is opening a context menu where you should select *„create a new experiment"*, give it a name and continue.

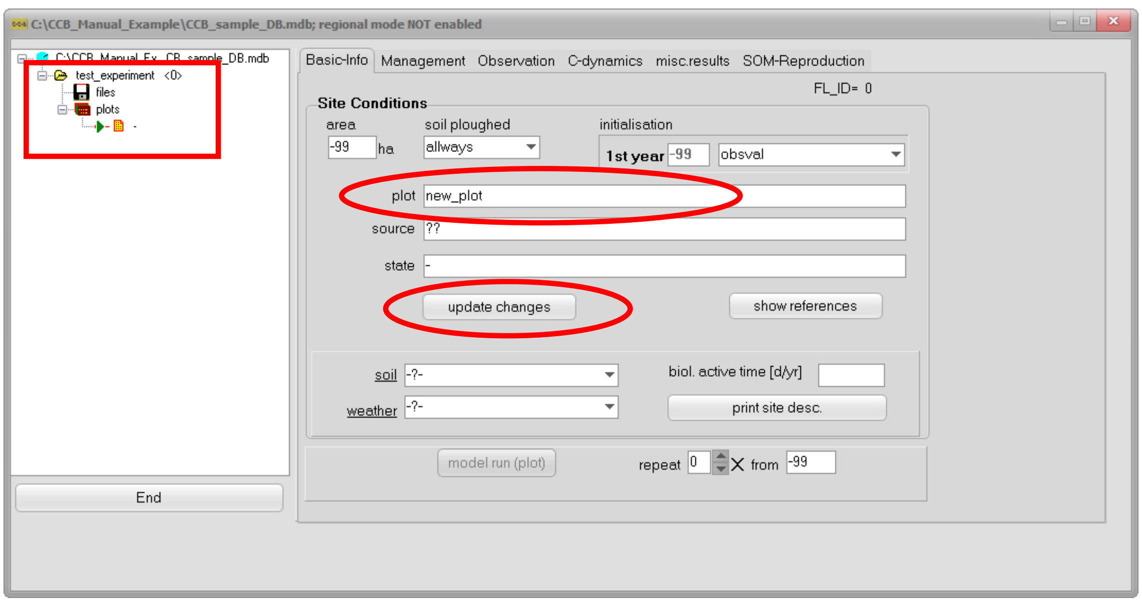


Figure 9: Editing a plot name

The new experiment is shown as folder containing already one plot. Click on the sheet-like pictogram to edit the data for this first plot. More plots can be added from the context menu (right click) of the plots symbol. The model results depend on the items soil, weather, the selection of the initialisation mode, and the selection of the tillage option (soil ploughed) – all other fields in this tab are only for the description. The plot name will be shown in the tree view at the left side of this form.

2.3.2 Soil data

You have to select the soil data for your corresponding plot in the ‘Basic-Info’-tab of the ‘Plot Selection’. The drop-down menu will show you all soils stored in the CCB database. To add additional soils you can either directly use the database (see section ‘4 Input-/Output Parameters & Database’) or use the CCB internal tools.

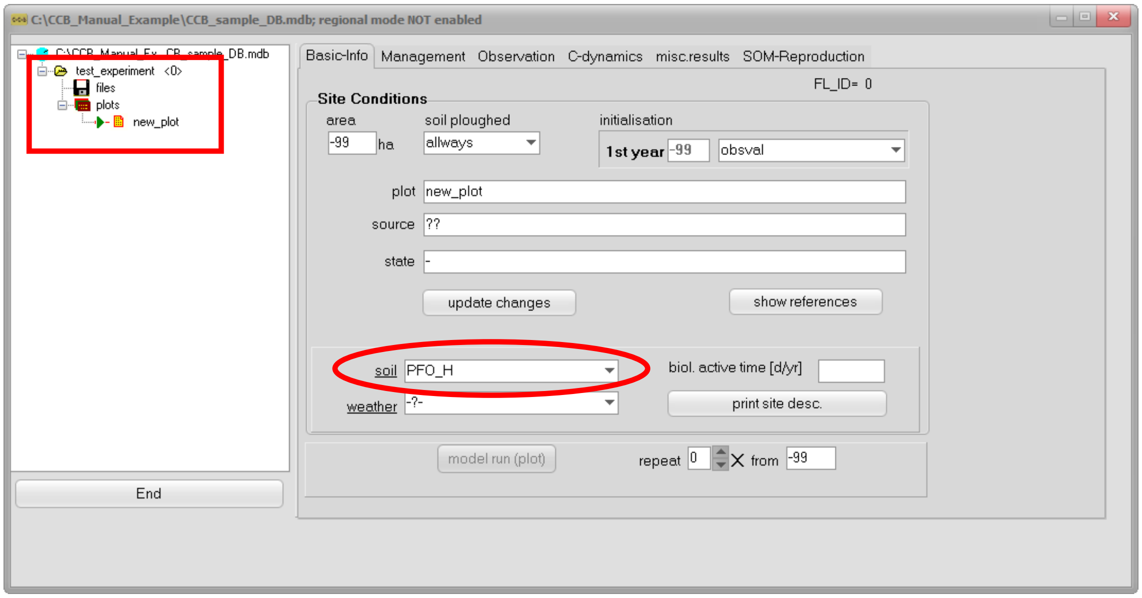


Figure 10: Selection of soil data

For using the CCB internal tools you can either double-click on ‘soil’ or go to the main menu, click ‘Parameters’ and select the ‘Soil Profiles’ tab. CCB needs some information about the uppermost soil layer 0-3 dm. All underlined items are necessary inputs all other parameters will be used by the model if specified from the user – otherwise the model is calculating estimates during the simulation run.

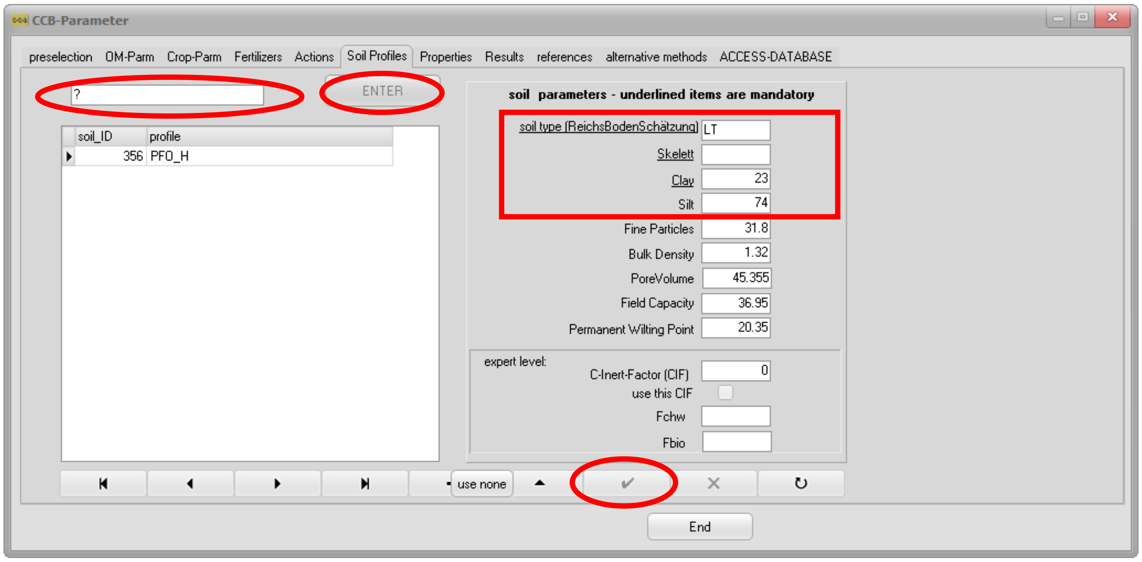


Figure 11: Creating new soil datasets

Enter the new soil name instead of the "?" and click on *„ENTER".* At finish the data should be saved clicking on the  button.

2.3.3 Climate data

Same as with soil data you have to select the climate data for your corresponding plot in the 'Basic-Info'-tab of the 'Plot Selection'. The drop-down menu will show you all climate stations stored in the CCB database. To add additional climate data you can either double-click on 'weather' or go to the main menu, click 'Climate data'.

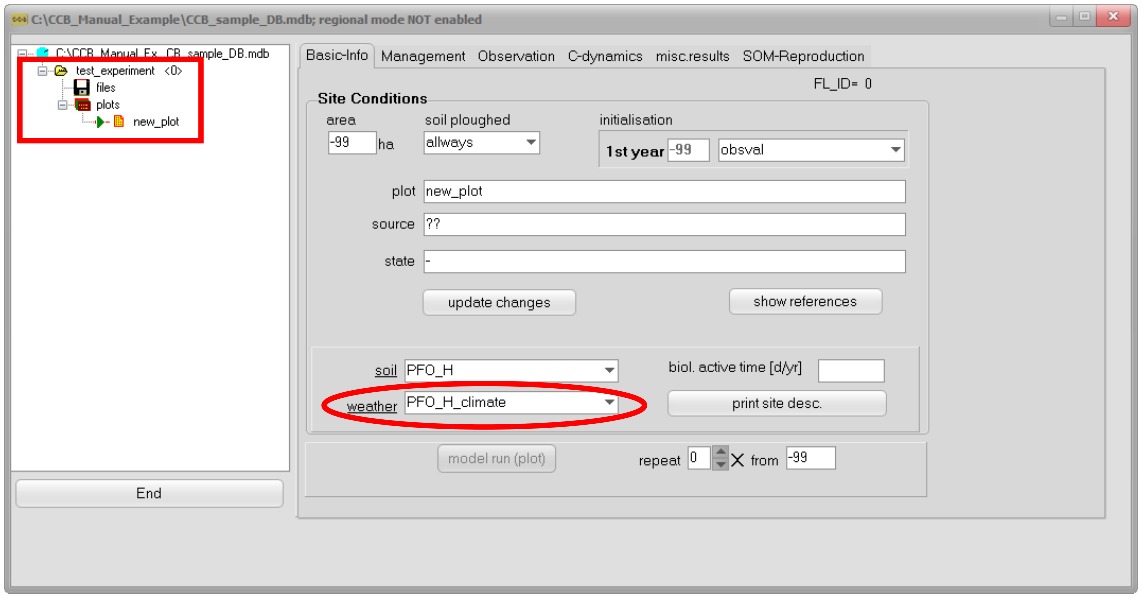


Figure 12: Selection of climate data

The climate data is stored separately and can be assigned to any plot. CCB is able to use climate data (annual rainfall and average air temperature) for each year or only one record as long term average. The last case is indicated using the year 0. Start editing with a new name for this site and click on "*create new station*".

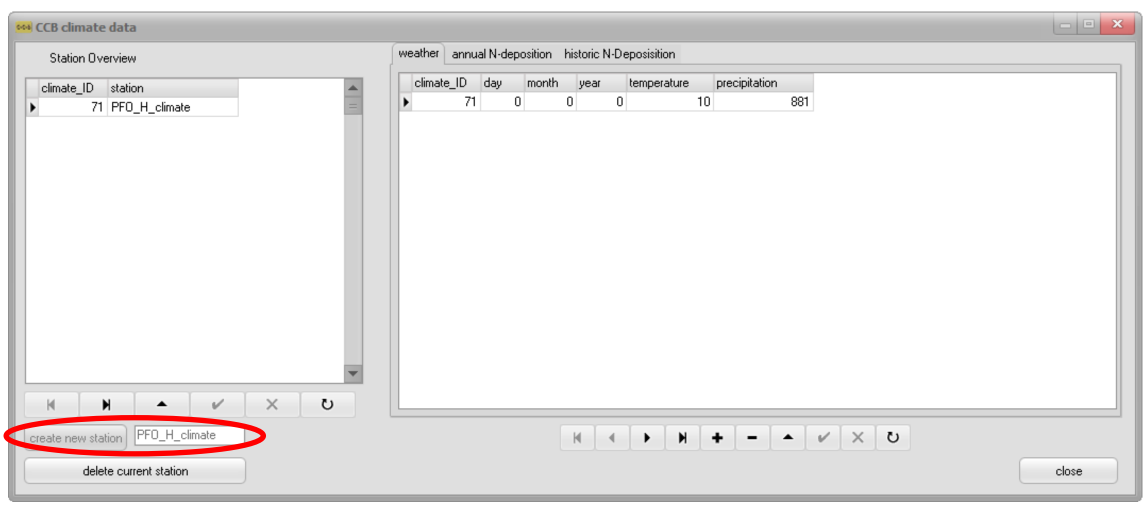


Figure 13: Editing climate records

With the 3 tabs ‘weather’, ‘annual N-deposition’ and ‘historic N-Deposition’ following climate information can be edited:

climate_ID	Unique value	[-]
station	Name	[-]
temperature	Annual average	[°C]
precipitation	Annual sum of precipitation	[mm]
N_dep_y	Annual N-deposition	[kg ha^{-1} a^{-1}]
basic year	First year to start calculated N-deposition	[-]
N-dep(basic)	Initial value of N-deposition	[kg ha^{-1} a^{-1}]
final year	Last year to finish calculated N-deposition	[-]
N-dep(modern)	Final value of N-Depositions	[kg ha^{-1} a^{-1}]

The input of N-deposition has only an impact on the calculation of N-balances and is not used during simulation of SOM turnover.

2.3.4 Management data

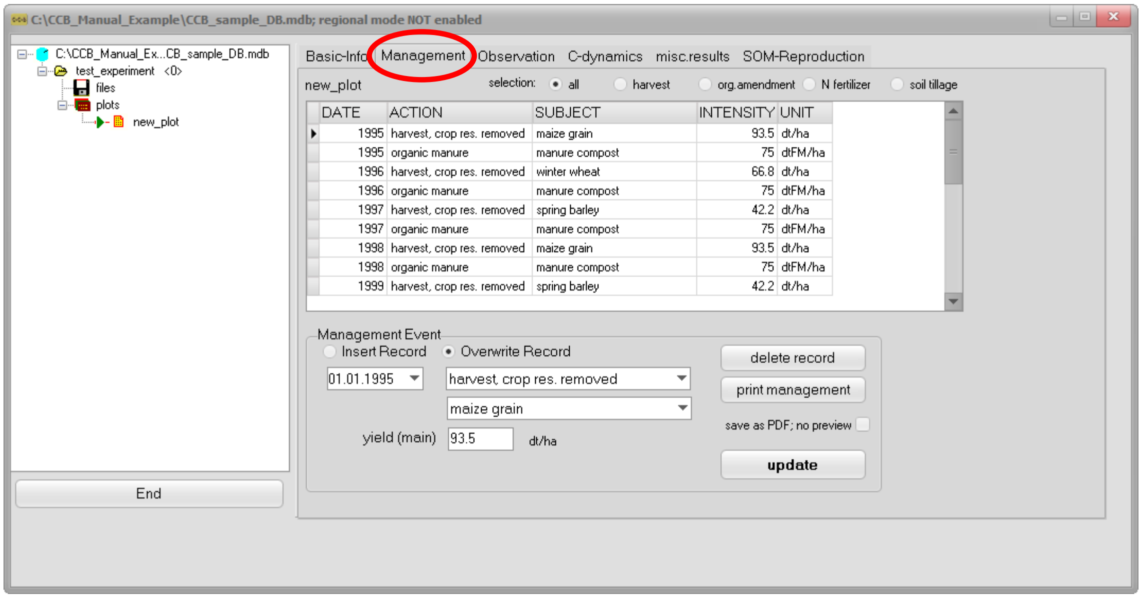


Figure 14: Editing management data

The Management-sheet is a compilation of management events for the selected plot. In the lower part of the form you can edit every single „Management Event“:

Insert Record: The record is added to the database

Overwrite Record: The current record is changed

Date: Only the year is significant – if known day and month can be given to have a better documentation

Event description: - Please select first the appropriate event from the upper dropdown menu („*harvest, crop res. removed*“, „*organic manure*“, „*mineral N fertilizer*“, “*irrigation*“, „*harvest, crop res. ploughed*“ and (in ‘regional mode’) “*reduced tillage*”)
- after that please select the related object (crop, fertilizer …)
- and finally edit the intensity (yield or amount).
- When using the ‘regional-mode’ also the regional share of the affected area of an management event has to be defined using the item “FLA%” (for further details see section ’2.6 Special application cases’).

delete record: Only the current record is deleted

print management: Output of management data on printer or as PDF-file

It is important to select the proper harvest mode: “crop res. removed" means that all by-products are removed together with the main product while “crop res. ploughed” means that e.g. straw is left on the field (only not coupled with a ploughing event if the tillage option is turned on).

You can copy the management data from one plot to another plot using drag'n drop. First activate the 'source' plot and open the management tab. Point with the mouse on the source plot, hold shift and start dragging the plot symbol to drop it onto the 'destination' plot. During this operation the mouse pointer will change to give you some assistance.

2.3.5 Observations

CCB works with data about C_{org} (mandatory) and some other optional indicators like N_t (see following table). All can be selected using the drop-down menu. C_{org} and N_t dynamics require to specify an initial value checking the box. This will set the year number to 0. If there is a soil sample from the same year that should be used for model assessment it will have the year number 1.

N_t	total soil nitrogen	[M%]
mic.biom. C	C in microbial biomass	[µg/g]
organic Carbon (C_{org})	total organic carbon	[M%]

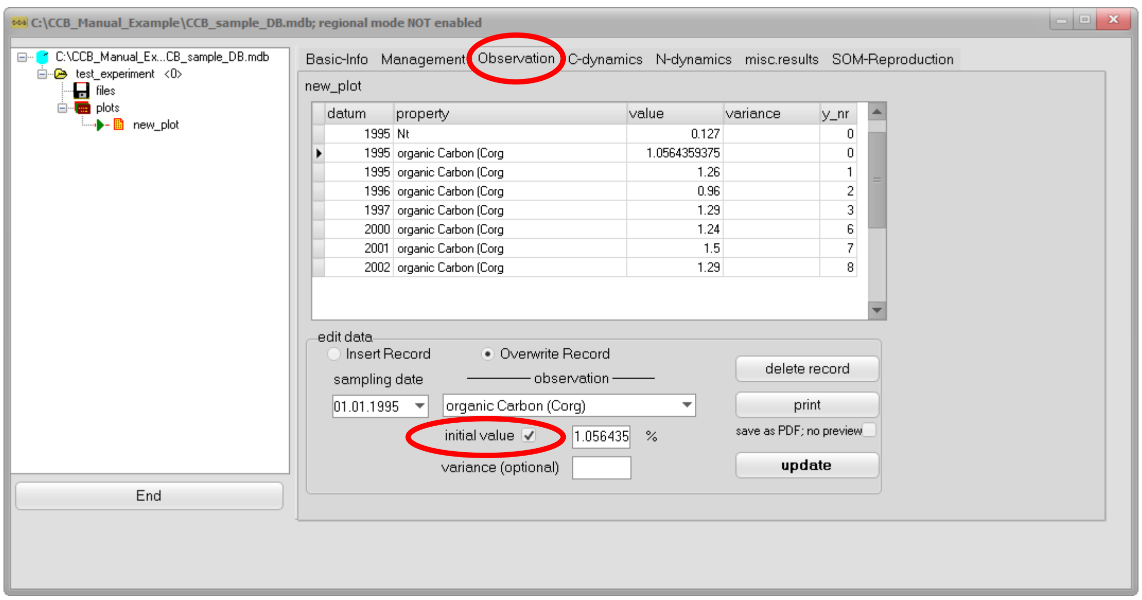


Figure 15: Editing observation data

Also in this sheet you find the Options *„Insert Record"* and *„Overwrite Record"* as well as following items:

sampling date:	Only the year is required day and month are ignored by the model.
observation:	Select the category
initial value:	Only one is allowed for N_t and C_{org}
variance:	Insert variance (optional)
print:	Print or send the data to a PDF-file

2.4 Editing parameters

2.4.1 Overview

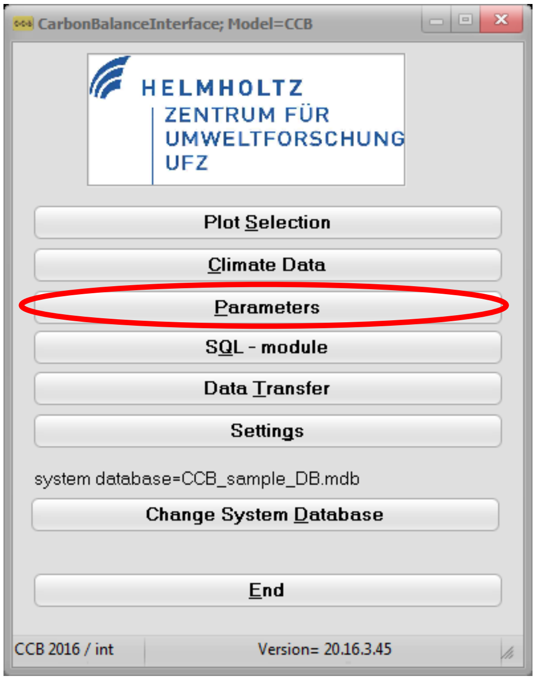


Figure 16: Start editing parameters

Go to the main menu and select „Parameters“ to start the editing of model parameters. You find a collection of sheets for different parameter types. There are two kinds of sheets: sheets containing adaptable parameters and sheets showing model parameters which are not changeable, thus just for your information. The sheet “ACCESS-DATABASE” is providing you access to the complete datasets of the model database.

preselection: select parameters which shall be shown in the dropdown menus of the management parameterization

OM-Parm: parameterization of organic matter: residues & org. substrates

Crop-Parm: parameterization of crops

Fertilizers: parameterization of mineral fertilizers

Soil Profiles: parameterization of soil profiles (top soil, 0-30cm)

Properties: list of selectable observations to be used for model assessment (helpful to directly read the database table “measurements”)

Actions: list of selectable management actions with their item_ix (helpful to directly read the database table “cultivation”)

Results: overview over aggregated model results (error analysis and N balance)

ACCESS-DATABASE: access to the complete model database

2.4.2 Preselection

Within the sheet “preselection” you have the possibility to select (-1) and unselect (0) management options. You can either double-click on an item to change the selection status or manually type in the desired option (-1 or 0). Management options that are unselected will not be shown in the dropdown menus of the management parameterization of your plots (plot selection). This is especially handy if you have a large collection of management options.

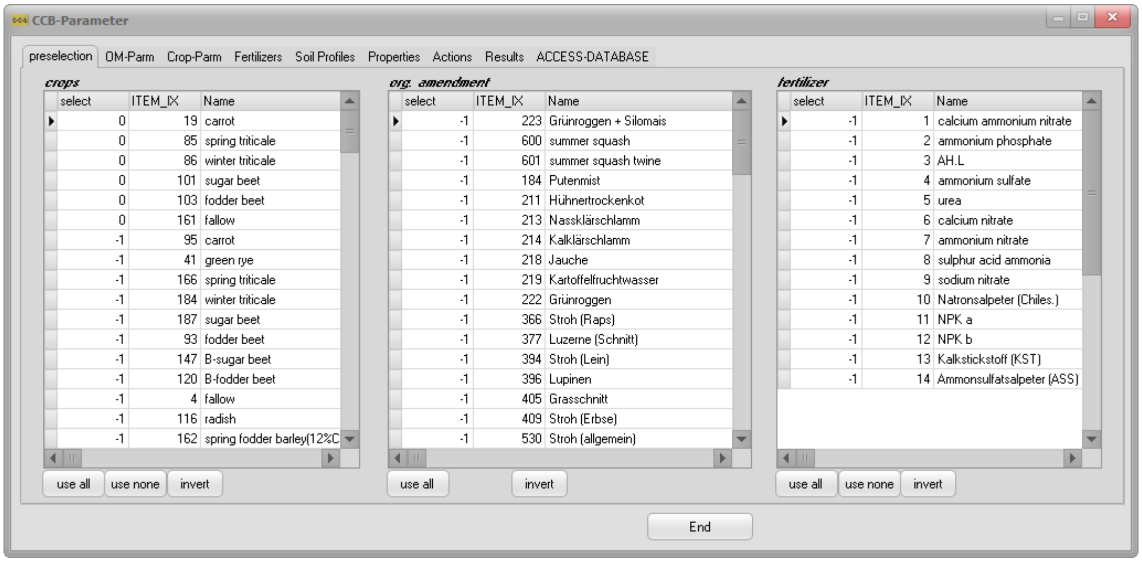


Figure 17: Preselection of management options

2.4.3 Organic matter, crops, fertilizers & soil profiles

Within the following sheets model parameters are easily adaptable by typing the new values into the corresponding fields. For a description of the individual model parameters please see the sections ‘3 Theoretical Documentation’ and ‘4 Input-/Output Parameters & Database’.

2.4.4 Results

The ‘Results’ sheet gives an overview on aggregated model results (error statistics and N-balance).

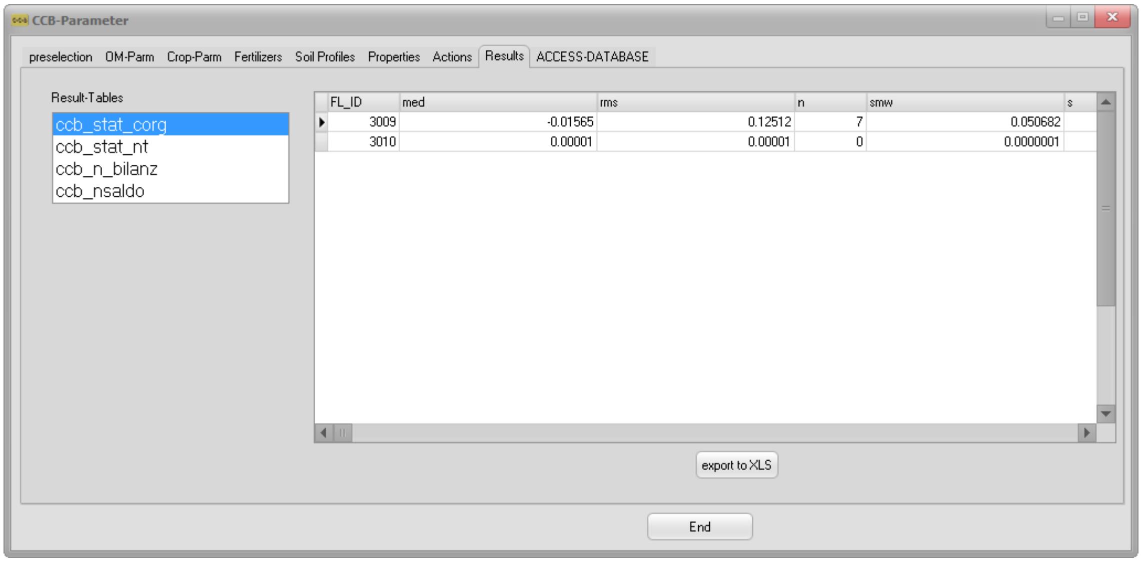


Figure 18: Results sheet

Error statistics

The error statistics statistics for C_{org} and N_t simulations can be (re)calculated for all datasets using the context menu of the database in the tree-view of the form „plot selection":

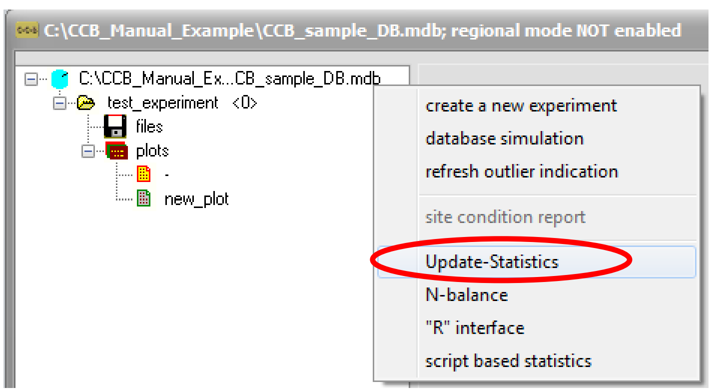


Figure 19: (Re)calculate error statistics

The results are stored in the tables '*ccb_stat_corg*' and '*ccb_stat_nt*'. In many cases an export to Excel may be helpful for further using these results.

FL_ID	unique plot identifier
med	mean error (error = residue= difference between model and measurement)
rms	root mean square error
n	record count
smw	standard error of the residues ($\sqrt{\sigma^2/n}$)

s	standard deviation of the (hypothetical) normal distribution of residues (square root of variance)
rele	med (mean error) related to observation mean of the plot
r_krit	least significant r value (as reference)
r_sim	correlation between observation and simulation results
r_dif	correlation between med (mean error) and time
ef	model efficiency
rmsprz	relative root mean square error
medprz	relative mean error (residues related to each single observation)

only for Corg for a detailed assessment a decomposition of the mean standard deviation of the residues following H.G.Gauch, J.T.G.Hwang G.W.Fick (2003): Modelevaluation by comparison of model-based predictions and measured values. Agron. J. 95:1442–1446

SB	squared bias
NU	non unity slope
LC	lack of correlation

N-balance

The context menu of the database in the tree-view of the form „plot selection" provides the opportunity to (re)calculate the nitrogen balance for two different viewpoints. During the calculation several tables are filled with data.

Table '*ccb_n_bilanz*' (annual balance elements):

FL_ID	plot identifier
year	balance time step
idx	unique indicator: str(FL_ID) + "_" + str(year) (plot_year)
	sources
N_m_om	N mineralisation/imobilisation from turnover of organic compounds (SOM &FOM)
N_Org_inp	total N input with organic amendments (manure, compost etc.)
N_kop_inp	N input with by-products left on field
N_SAAT	seed bound N input (table N_SAAT_IMP)
n_dng	N-input with mineral fertilizer
n_bindung	symbiontic N fixation of legume crops (table LEG_PARM)
n_deposition	atmospheric N.deposition (from climate data)
asym_nbind	asymb. N-fixation (depends on application rate of min. N.fert.)
	sinks
N_EWR	N uptake of the crop residues (stubble+root)
n_entz	total N-Uptake by crop (main + by-product)

Table ‘*ccb_nsaldo*’ (average data over the whole time interval):

FL_ID	plot identifier
n_mindg_inp	N-input with mineral fertilizer
n_orgdg_inp	total N input with organic amendments
n_mos_inp	Nflux from turnover of organic ccompounds (SOM&FOM)
n_leg_inp	symbiontic N fixation of legume crops
n_asym_inp	asymb. N-fixation
n_depos_inp	atmospheric N.deposition
n_saat_inp	seed bound N input
N_gratis	n_bindung + asym_nbind + n_deposition + n_saat
n_ewr_upt	N uptake of the crop residues (stubble+root)
n_HUKP_upt	total N-Uptake by crop (main + by-product)
n_saldo_soil	(N_gratis) - (n_entz+n_ewr)
n_saldo_plot	(n_org_inp + n_dng + N_gratis) - (n_entz)

The final balance tables that are shown in the interface are: ‘*Nmin_saldo*’ and ‘*NT_saldo*’:

Table ‘*Nmin_saldo*’: balance of the fluxes related to the N_{min} pool neglecting the N losses (average data over the whole time interval):

FL_ID	plot identifier
n_pflanze_out	total N-Uptake by crop (main + by-product)
n_mindg_inp	N-input with mineral fertilizer
n_mos_ inp	Nflux from turnover of organic ccompounds (SOM&FOM)
n_leg_inp	symbiontic N fixation of legume crops
n_asym_inp	asymb. N-fixation
n_depos_inp	atmospheric N.deposition
n_saat_inp	seed bound N input
saldo_nmin_soil	(N_mineralised + N_gratis) - (N_entz + N_ewr)
anz	aggregated years

Table ‘*NT_saldo*’: balance related to the total nitrogen stock in the topsoil of a field, neglecting the N losses (average data over the whole time interval):

FL_ID plot identifier

n_abfuhr N offtake from field: n_entz - n_kop_inp

n_mindg_inp N-input with mineral fertilizer

n_orgdg_inp total N input with organic amendments

n_leg_inp symbiontic N fixation of legume crops

n_asym_inp asymb. N-fixation

n_depos_inp atmospheric N.deposition

n_saat_inp seed bound N input

n_saldo_plot (n_org_inp + n_dng + N_gratis) - (n_entz)

2.4.5 Access-database

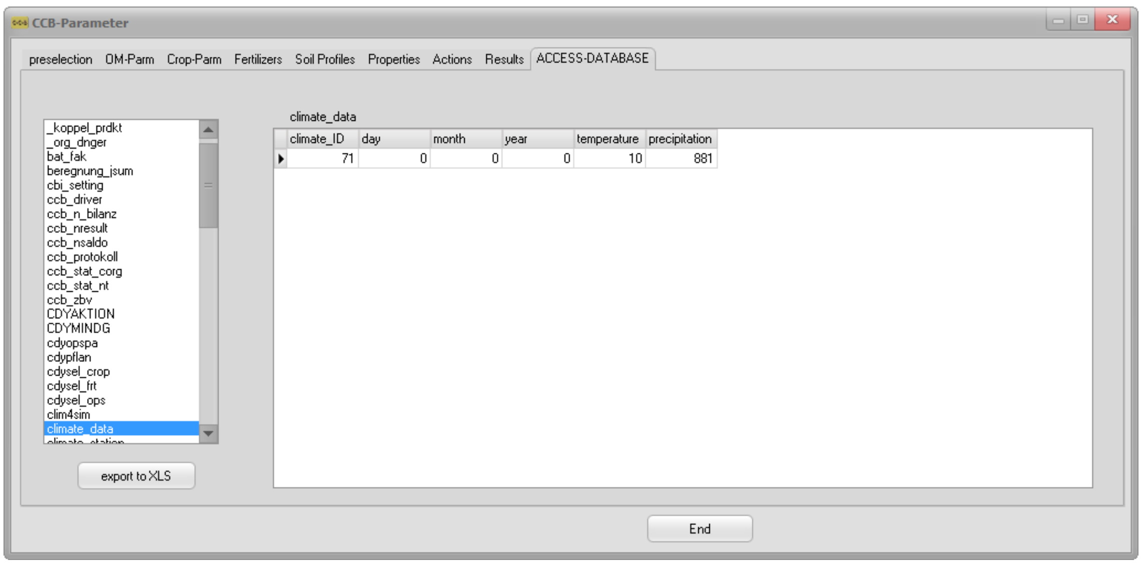


Figure 20: Access to the complete model database

The sheet 'ACCESS-DATABASE' gives you access to the complete model database. First double-click on a dataset then right-click on a record and use tab to navigate through the data. To change values: move to the item (background is yellow), press ENTER (background is blue, complete item is selected), click on the item (background is white) and start editing single symbols.

2.5 Simulation & result presentation

2.5.1 Start simulation runs

Choose the *„Basic-Info“* tab and click *„model run (plot)*” to simulate one selected plot.

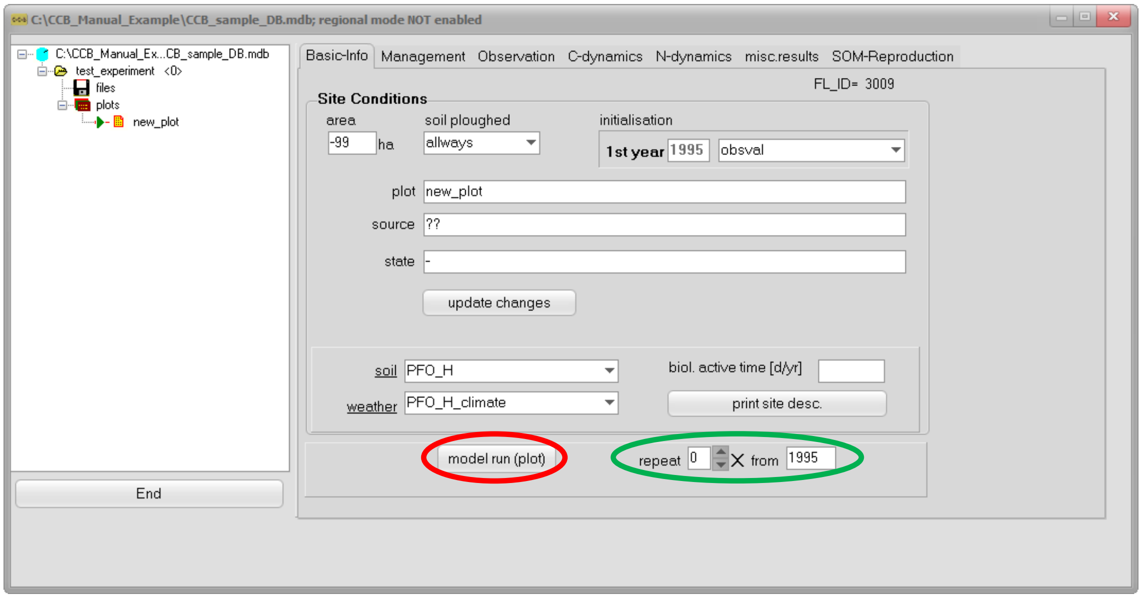
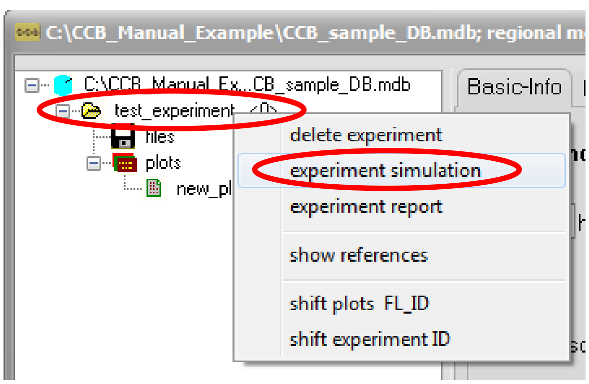


Figure 21: Start simulation of the selected plot

It is possible to simulate a certain management in a circular mode without entering the same data for each year. This repetition mode requires the number of cycles and the year where the repeated cycle should be started (Figure 21, green circle).

Furthermore it is possible to simulate one complete experiment (all plots: *„experiment simulation“*) or the complete content of the database (*„database simulation“*).



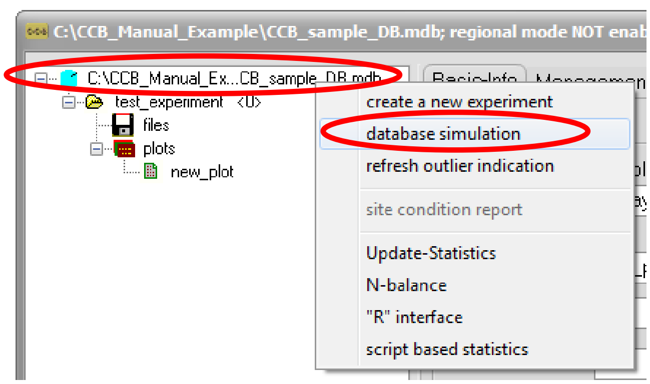


Figure 22: Select simulation of one complete experiment (left) or the complete database (right)

If appropriate, it is possible to repeat the management scenario several times starting at a given year. This may reduce the effort for data input especially for general problems for instance if a cropping system can only be described with yield data that are constant over time.

When a database simulation or experiment simulation was selected an additional screen will allow you (un)select plots, which will be simulated:

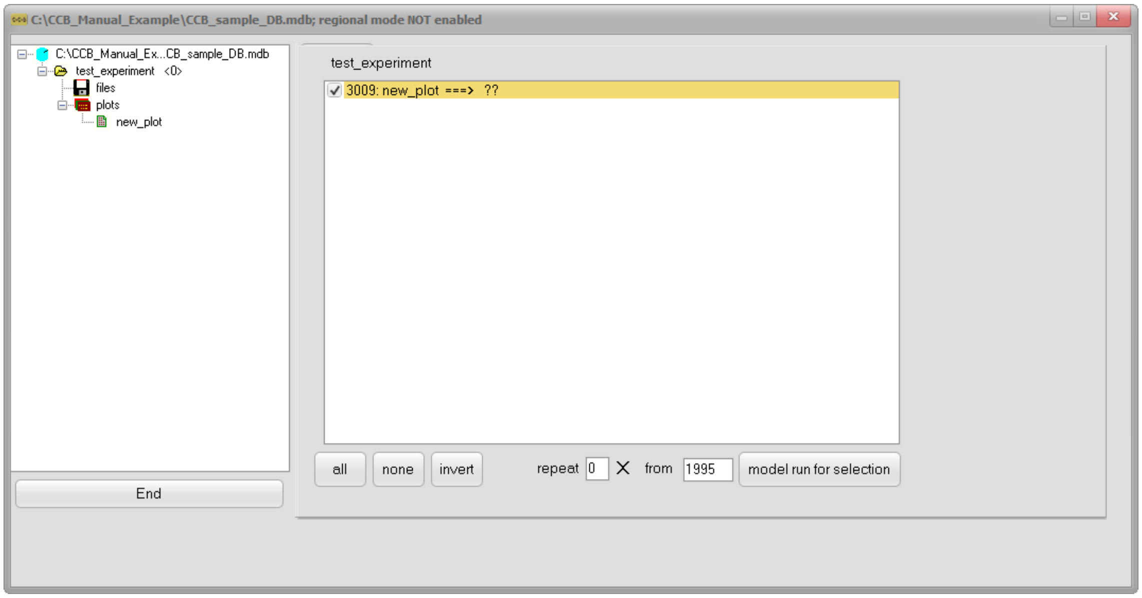


Figure 23: Stat simulation run of one complete experiment or the complete database

The run button brings up the simulator form that shows all selected plots for this simulation run. Please click the „*calculate*“ button to proceed (only necessary when simulating an complete experiment or database).

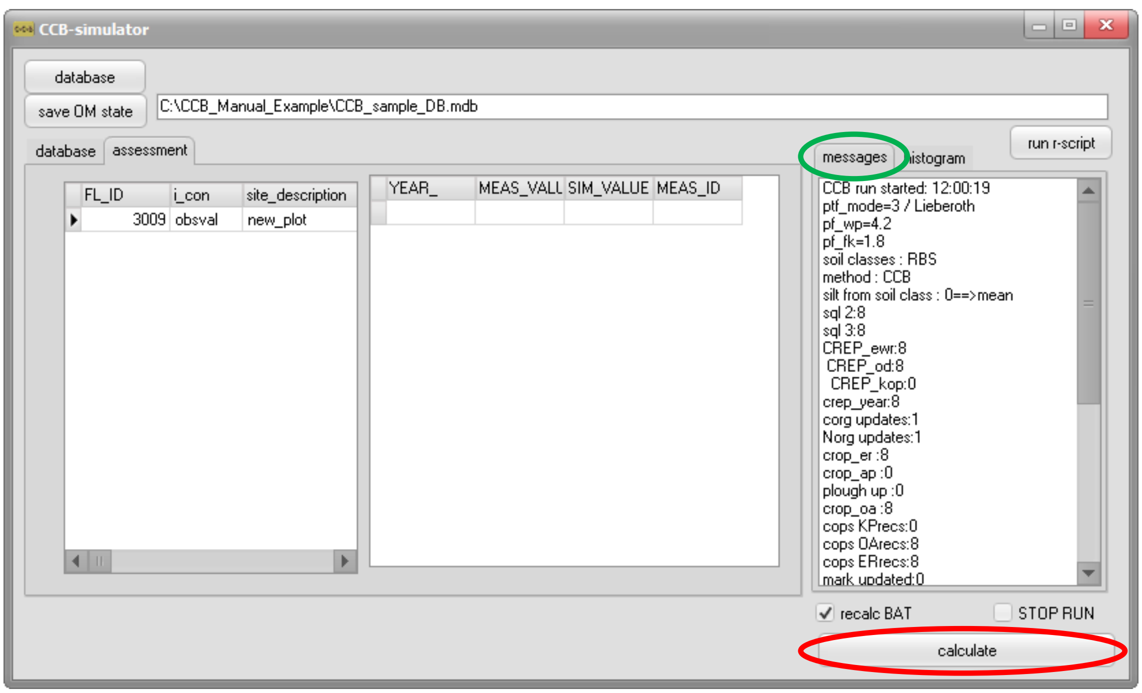


Figure 24: Summary screen of a simulation run

During the run you can see messages from the model that may help to identify possible errors in the input data (green circle, Figure 24).

2.5.2 Checking results

After finishing the simulation we go back to the user interface and may view the results in the appropriate sheets as a simple graph together with some statistics. These can also be reported (printer or PDF file) or exported (XLS file).

The sheets ‘C-dynamics’, ‘OM-turnover’, ‘N-Dynamics’ and ‘micr.BM’ are presenting the results of the simulation run with respect to C_{org}, N_{org} and C in microbial biomass respectively (only if observation values are available). Measured values are considered for the statistics and the plot as well. Outliers will be shown as red triangles if the option for outlier identification has been activated from the context menu of the database.

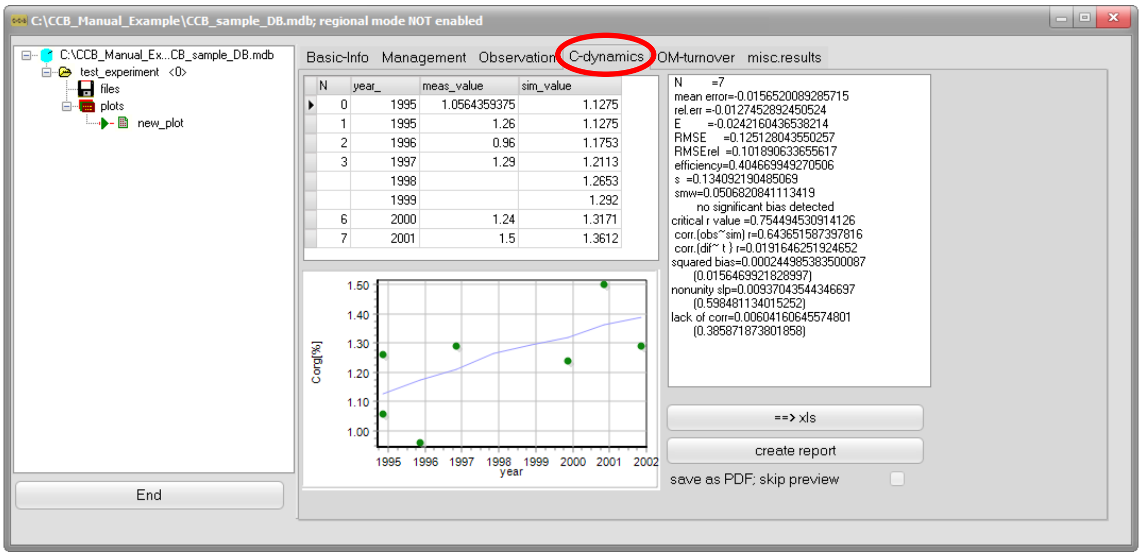


Figure 25: Presentation of results (C-dynamics)

While the sheet ‘C-dynamics’ is presenting the temporal development of C_{org}, the sheet ‘OM-turnover’ is given an overview about carbon fluxes:

Column name	Plot selection	Description	Unit
SOM gain	SOM reproduction	C_{org} input from FOM to SOM	kg C / ha / a
SOM loss	SOM decomposition	C_{org} loss from SOM to CO_2	kg C / ha / a
saldo	SOM saldo	SOM balance = C_{rep} - C_mineralisation	kg C / ha / a
CO2 prod.	total C emission	total carbon loss from SOM and FOM to CO_2	kg C / ha / a
soil C storage	total C in soil	total C in soil from all SOM pools	t / ha
BAT	BAT	biologic active time	d / yr
REP_IX	REP_IX	SOM reproduction index = C_{rep} / BAT	-

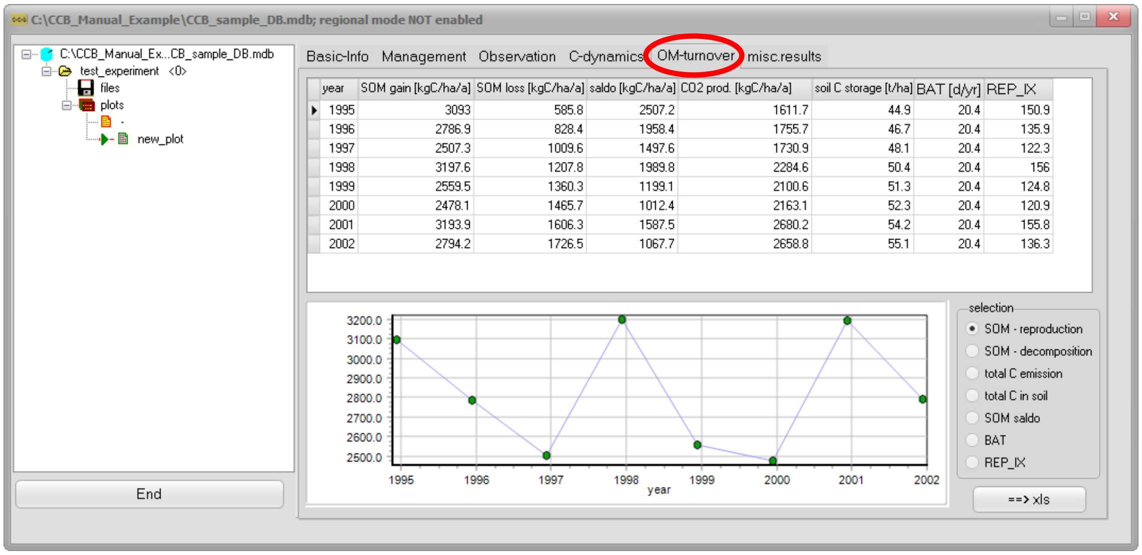


Figure 26: Presentation of results (OM-turnover)

Within the sheet ‘misc. results’ a collection of different outputs is presented. For more information on the individual outputs please also see the sections 3 (Theoretical Documentation) and 4 (Input-/Output Parameters & Database):

Column name	Dropdown-menu	Description	Unit
n_m_om	N-mineralisation	N mineralisation from organic matter	[kg/ha/a]
n_ops	N in FOM	total N in fresh organic matter	[kg/ha]
C_ops	C in FOM	total C in fresh organic matter	[kg/ha]
c_som		total C in soil organic matter	[kg/ha]
n_som		total N in soil organic matter	[kg/ha]
c_lts	phys.stab. SOC	physical stable C in soil organic matter	[kg/ha]
cnr	CNR	cabon-nitrogen ratio	-
crep	C_rep flux	C reproduction flux from FOM into SOM	[kg/ha/a]
bat	BAT	biological active time	[day]
bd	BD	bulk density	[g/cm³]
pwp	PWP	permanent wilting point	[VOL %]

2.6 Special application cases

2.6.1 Indicator based simulation

A common problem of applications on meso to large scale is the availability of reliable information about the initial C_{org} concentration. One option is here to leave the quantitative calculation of the C-dynamics and not provide information about initial C_{org}. In this case the model calculates the indicator Rep_IX that includes the soil carbon reproduction as well as the site conditions for an assessment of the management.

2.6.2 Simulation of a pre-treatment

If an experiments starts with considerable changes of the management it may be reasonable to include the history of this place in the simulations. In this case it is possible to simulate the history (i.e. as pre-treatment) in a separate plot of the experiment and enable the scenario option within the "*settings*".

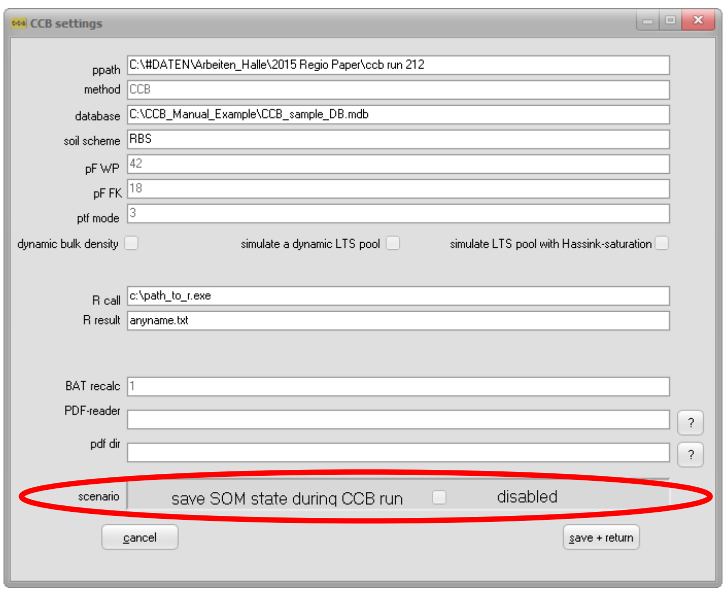


Figure 27: Possibility to enable the scenario option for simulation of a pre-treatment

The soil condition after this pre-treatment is stored in the tables 'som_state' and 'fom_state'. This data can be used as initial condition for other plots under the pre-condition that the last year of the pre-treatment simulation is just prior the intended start of the scenario simulation. The plot with the pre-treatment can be selected as initial condition instead of "obsval" or "null":

Figure 28: Set a pre-treatment as initial condition

A pre-management can also be helpful if no initial value for C_{org} is available. Some pre-management like a standard crop rotation may be applied for a long time interval. This pre-management itself requires an initial value but the longer the pre-management is simulated the lower is the impact of this initial C_{org} on the results of the actual scenario.

2.6.3 Regional-Mode

The ‘regional-mode’ was developed for meso to large scale studies, where crop rotations are not available. Within the Regio-CCB modification crop share statistics can be used as data input instead of crop rotations. Furthermore also the share of conservation tillage and conventional tillage can be considered. Input of crop shares and tillage shares can be parameterized on an annually basis.
To activate the ‘regional-mode’ right-click on your database within the ‘Plot Selection’ and then click on ‘regio mode’. When the ‘regional-mode’ is activated the additional item (“FLA%”) will be available in the management parameterization (see also section ‘2.3.4 Management data’). The “FLA%” item is defining the regional share of the affected area of an management event, e.g. the regional share of a cultivated crop.

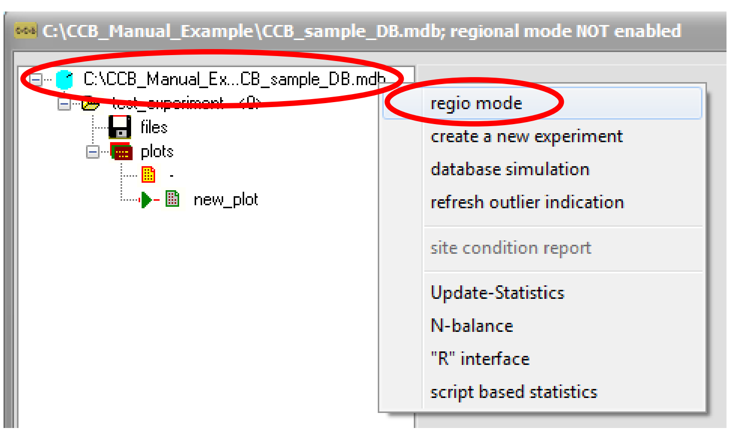


Figure 29: Activation of the ‘regional mode’

The ‘regional-mode can only be activated for a complete database. It is recommended to back-up your database before doing so. Furthermore please consider to check your management parameterization of already existing plots. The 'regional-mode' has a different theoretical concept in the parameterization of the agricultural management.

2.6.4 Using the batch mode

CCB can be started from the command prompt as well. In this case the program call has to be complemented by a selection of following options / parameters (not case sensitive):

GO	automatic start of simulation run
RC= <repletion count>	number of cycles
TC=< initial year>	cycle loops back to this year
PPQ=<preprocessing sql script>	useful to select several plots to be simulated
POQ=<postprocessing sql script>	useful for automated result processing
ID=<unique plot identifier>	recommended if a single plot is simulated
DB=<mdb file >	name of the database incl. complete path
NW or !	exit from application after finishing the simulation run

Further options may be available for special applications - please contact the developer.

If the model is used in batch mode it is simulating all plots that are marked with status=1 in the table 'site_state' (see section '4 Input-/Output Parameters & Database'). This behaviour can be used to start the model for a number of plots. In this case it is recommended to provide an appropriate SQL script over the PPQ parameter.
Following an example for starting CCB in batch mode:

```
ccb.exe DB= CCB_sample_DB.mdb PPQ1=use_none.sql PPQ2=use_all.sql go !
```

with 'use_none.sql':

```
UPDATE field_description INNER JOIN site_state ON field_description.FL_ID = site_state.FL_ID SET site_state.status = 0
```

and 'use_all.sql':

```
UPDATE site_state SET site_state.status = 1 WHERE (((site_state.FL_ID)>0));
```

2.7 Known problems

There may be some adaptations required to make CBB running properly. If you edit the data with the CBB interface it is recommended to use a decimal point as decimal symbol because all data changes are made via SQL which is using the semicolon as list separator! Furthermore it is recommended to have a short date format as dd.mm.yyyy. These settings can be customized or checked at the MS-Windows Control Panel under “Region and language” (German: Systemsteuerung “Region und Sprache”) and [Additional Settings/Weitere Einstellungen]:

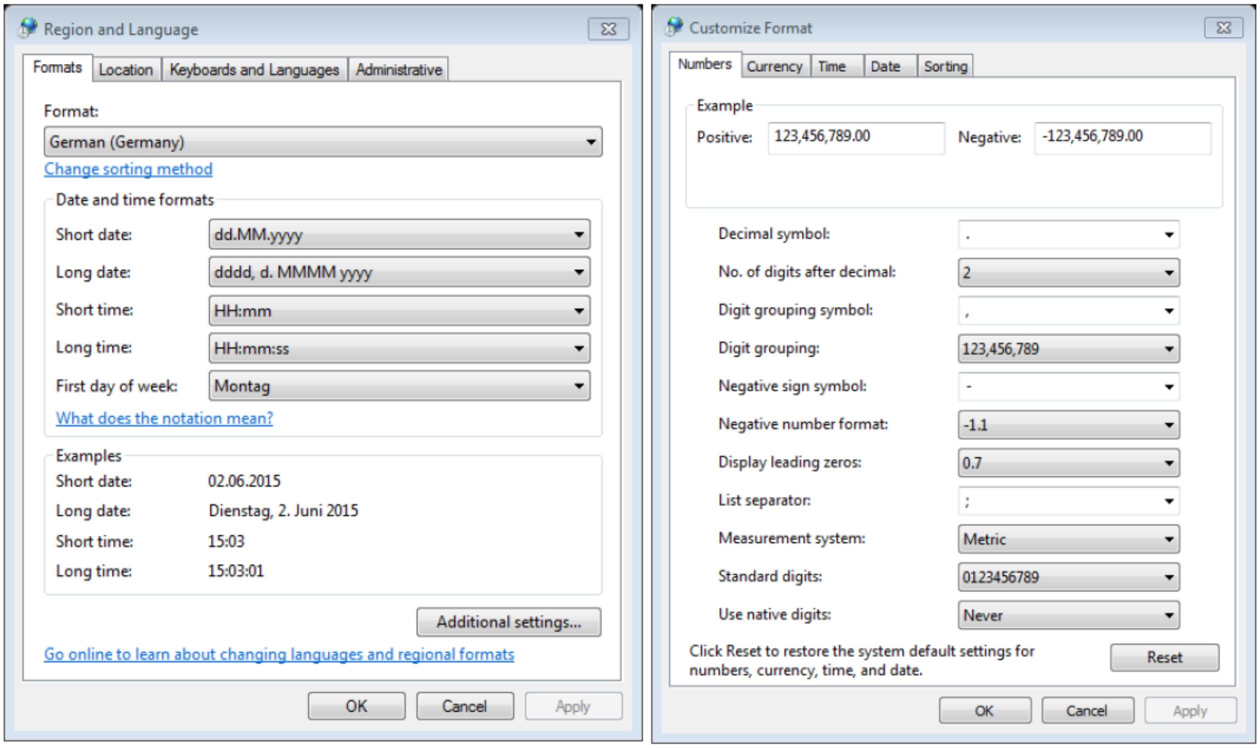


Figure 30: MS-Windows Control Panel “Region and Language” (left) to control the [short date/Datum (kurz)] entry and the [additional settings/Weitere Einstellungen] (right) to customize the [Decimal/Dezimaltrennzeichen] and [Digit grouping symbol/Symbol für Zifferngruppierung]

If required, the user may change the settings in the registry database of the windows system. Therefore you need to start the program regedit.exe that is localized in the windows folder. The information is stored under

- HKEY_CURRENT_USER/Software/ccb

If changes are necessary users should proceed very carefully to avoid problems with the CCB model.

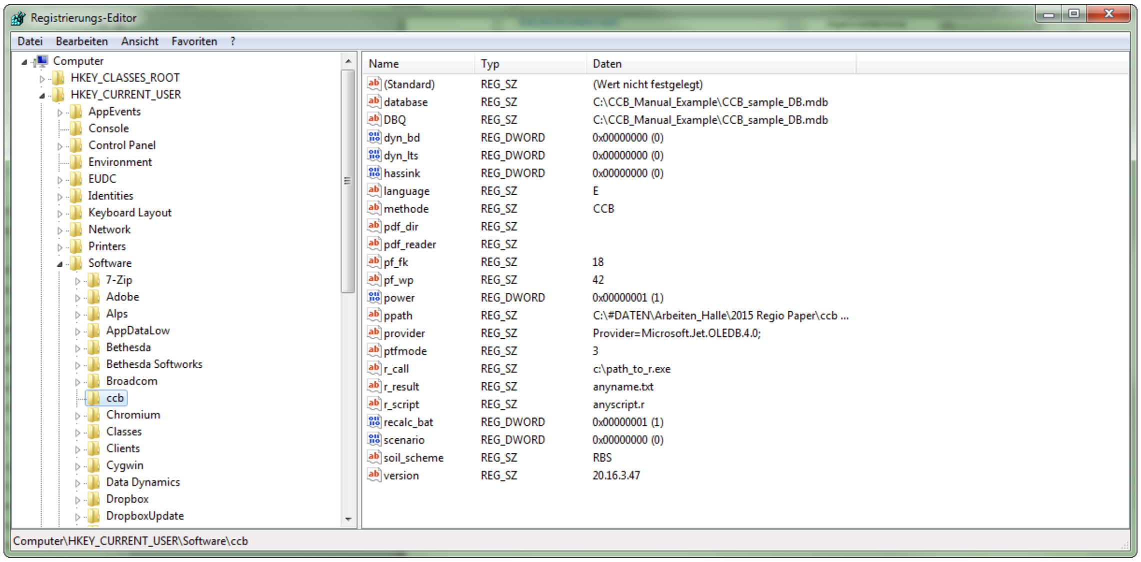


Figure 31: Registry Editor with the keys for the CCB model

3 Theoretical Documentation

3.1 Model structure

The general construction of the CCB model is shown in Figure 32. The used pools are the same as in the CANDY model (Franko, 1989; Franko et al., 1995). SOM is divided into an active pool (A-SOM), where the mineralization takes place, a stabilized pool (S-SOM) representing the passive but decomposable part of the SOM and a long term stabilized pool (LTS-SOM) that is here taken as inert. Beside SOM there are a number of FOM pools that are characterized by the origin of organic matter (OM).

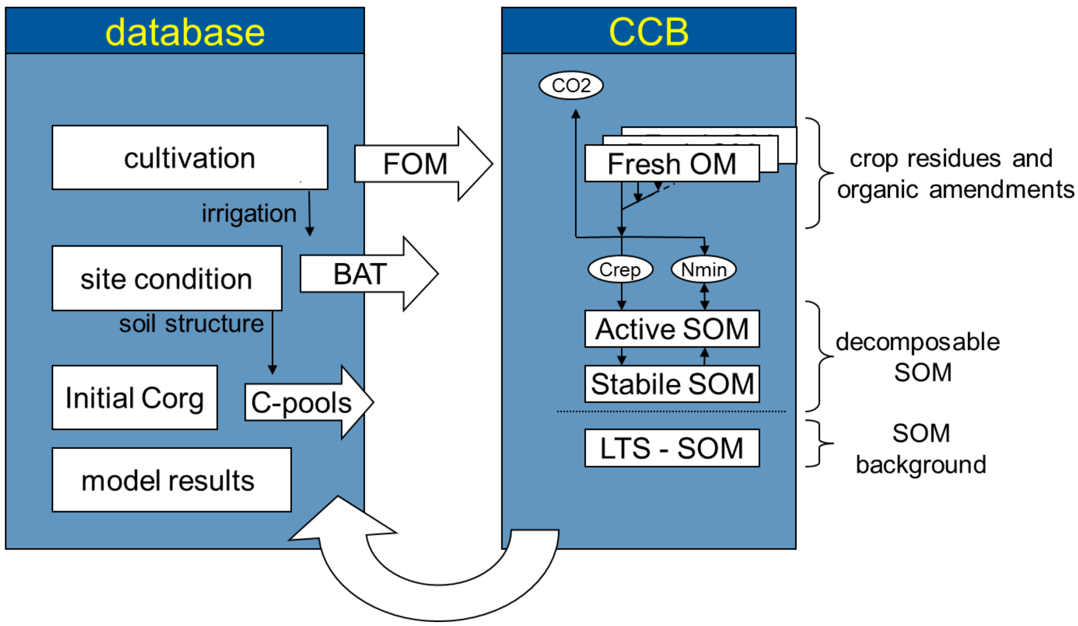


Figure 32: CCB general approach

The modelling of turnover kinetics is based on first order kinetics. The used time variable *t* is the Biological Active time (BAT) according to the concept used in CANDY (Franko et al., 1995, Franko and Oelschlägel, 1995). BAT is calculated as annual value according to the air temperature, the amount of rainfall plus irrigation water and the soil texture (content of fine particles < 6.3 micrometers, including clay and fine silt). In order to provide information about nitrogen mineralization the model must be able to describe the interaction between SOM turnover and nitrogen fluxes connected with the turnover of the FOM pools and the mineralisation of the active SOM.

The state variables for the pool sizes in the model have the dimension of mass unit per area unit – usually kg ha^{-1} which is equal to 10^{-1} g m^{-2}. The observation data for carbon and nitrogen storage in soil are often available as concentration (ppm or M%) in the fine soil material (< 2 mm grain size). Therefore the model results are presented as concentration using the bulk density, gravel content and the depth of the top soil layer to transform the units. Generally a top soil layer of 0.3 m is assumed. The conversion between mass (*M*) and concentration (*CONC*) of any pool is accomplished according to the following equation (Eq. 1):

$$M = CONC \cdot \rho_B \cdot h \cdot \left(1 - \frac{GC}{100}\right) \cdot 10^4$$ Eq. 1

M:	pool mass in g m^{-2}
CONC:	matter concentration in %
ρ_B:	bulk density in g cm^{-3}
GC:	gravel content in %
h:	depth in m

SOM dynamics are usually explored by C_{org} observations but because its close relation to soil nitrogen the C/N ratio is often used to additional characterize the SOM. Therefore the model description includes relations to nitrogen fluxes and pool sizes.

Table 1: CCB input variables that pertain to conversions between mass and concentration

Variable	Definition	Unit	Name in database	Database table
ρ_B	soil bulk density	g/cm³	BD	soilproperties
GC	gravel content	%	skelett	soilproperties

3.2 Supply of fresh organic matter

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

a) organic amendments,
b) by-products that are left on the field after harvest and
c) crop residues such as roots and stubble.

The amount of FOM input from organic amendments (FOM_{oa}) is given in the scenario data and the carbon input C_{oa} can be calculated from the substrate specific parameters for dry matter content (DM_{oa}) and carbon content in dry matter (CC_{oa}).

$$C_{oa} = FOM_{oa} \cdot DM_{oa} \cdot CC_{oa}$$ Eq. 2

The FOM flux from the other both pathways has to be calculated as follows. The amount of by-products (FOM_{bp}) is calculated from the yield and a crop specific harvest index (HI):

$$FOM_{bp} = yield \cdot HI$$ Eq. 3

Knowing the FOM_{bp} amount the by-product related carbon input C_{bp} is calculated using the parameters for dry matter content (DM_{bp}) and carbon content in dry matter (CC_{bp}):

$$C_{bp} = FOM_{bp} \cdot DM_{bp} \cdot CC_{bp} \quad \text{Eq. 4}$$

The contribution from crop residues is also determined in relation to the crop yield calculating the size of the residual related N-pool (N_{res}) and the adequate C amount of the crop residues (C_{res}) from the substrate specific C/N ratio γ_{fom}:

$$N_{res} = F_{res} \cdot yield \cdot N_{cont} + K_{res} \quad \text{Eq. 5}$$

$$C_{res} = N_{res} \cdot \gamma_{fom} \quad \text{Eq. 6}$$

F_{res}. K_{res}, N_{cont}: crop specific constants describing the yield depending nitrogen amount of crop residues after harvest.

Table 2: CCB input variables that pertain to the supply of fresh organic matter

Variable	Definition	Unit	Name in database	Database table
DM_{oa} / DM_{bp}	dry matter content in fresh matter (substrate specific)	%	TS_GEHALT	cdyopspa
CC_{oa} / CC_{bp}	carbon content in dry matter (substrate specific)	%	C_GEH_TS	cdyopspa
HI	Harvest index (crop specific)	-	HI	cdypflan
γ_{fom}	C/N ratio (substrate specific)	-	CNR	cdyopspa
F_{res}	constants describing the yield depending nitrogen amount of crop residues after harvest (crop specific)	kg/dt	FEWR	cdypflan
K_{res}	constants describing the yield depending nitrogen amount of crop residues after harvest (crop specific)	kg/ha	CEWR	cdypflan
N_{cont}	Nitrogen content of crop residues (crop specific)	%	N_GEHALT	cdypflan

3.3 Quantification of site specific turnover conditions

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. In the CANDY model the calculation of the BAT interval includes the effects of soil temperature, soil water and soil aeration.

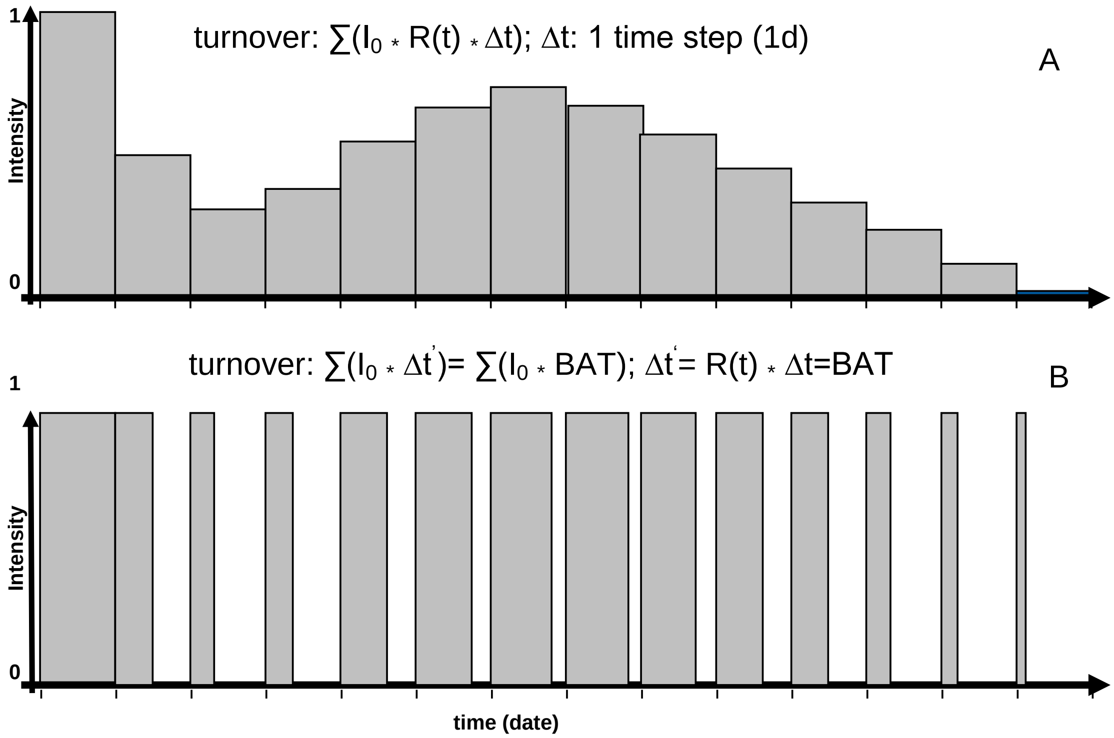


Figure 33: Schematic representation of the turnover calculation by the standard approach (A) and the BAT approach due to transformation of time steps (B).

The scheme in Figure 33 demonstrates the principle how different intensities of uniform time steps (Figure 33 A) are transformed into time steps of different length and uniform intensity (Figure 33 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 33 B). The CANDY model calculates BAT in daily time steps for each of the 3 top soil layers (0-3 dm). A more detailed description of BAT calculation can be found in the CANDY manual. For the CCB model we use only annual BAT sum as indicator for the potential turnover under the given conditions. Based on simulation results with the CANDY model a meta model for the annual sum of BAT was developed by Franko and Oelschlägel (1995) that considers soil texture and annual climate data (air temperature and rainfall) including the annual irrigation amount within the natural rain and an additional adaptation for conservation tillage.

The following R script may be the best way to explain this simplified BAT calculation as interpolation between different soil types:

```
BAT <- function(afat, ltem, nied) {
        a <- c(3.3541, 3.1825, 3.0629, 2.1824, 2.1698, 2.0054, 1.8676)
        b <- c(0.015698, 0.01325, 0.003204, -0.009797, -0.02726, -0.03232, -0.03178)
        c <- c(9.0870, 10.2234, 14.5547, 23.0218, 23.6263, 22.9473, 22.9300)
        fattab <- c(6.0, 8.0, 11.5, 15.0, 22.0, 32.0, 44.0)
        i <- 0
        nied <- min(nied_, 700)
```

```
        nied <- max(nied, 450)
        repeat {
                i <- i+1
                if ((afat <= fattab[i]) | (i==8)) {   break   }
                }
         if (i==1) {
                bat <- a[1] * ltem + b[1] * nied + c[1] }  else   {
                if (i < 8) {
                        i1 <- i-1
                        h1 <- a[i1] * ltem + b[i1] * nied + c[i1]
                        h2 <- a[i] * ltem + b[i] * nied + c[i]
                        p <- (afat - fattab[i1]) / (fattab[i] - fattab[i1])
                        bat <- (1 - p) * h1 + p * h2
                         }
                }
        if (i == 8)   {
                bat <- a[7] * ltem + b[7] * nied + c[7]
                }
        return(bat)
}
```

<u>*Adaptations of BAT for conservation tillage*</u>

We hypothesize that the reduction of the tillage depth leads to a stratification of SOM because of the missing soil mixing events. In order to acknowledge this effect, we hypothesize that the turnover activity is reduced in deeper soil layers. For ploughed soils this effect will be compensated by mixing the soil layers. If conservation tillage is applied the average turnover conditions should be reduced due to this depth depending reduction of turnover activity. Following the basic principles of the CCB model this effect has to be expressed as a changed value for the Biologic Active Time (BAT).
A reduction factor α was introduced that describes an exponential reduction of turnover activity of the next downward soil layer assuming a layer thickness of 1 dm.

$$\alpha = \exp(\sqrt{F_R \cdot F_D}) \qquad \text{Eq. 7}$$

The factor α depends on two components: a reduction due to reduced gas exchange F_D depending on soil texture that is here represented by the amount of fine soil particles < 6.3 µm (*FP*). The calculation of this factor is taken from the CANDY model as it has been described by Franko et al. (1997):

$$F_D = FP \cdot 0.2844 - 1.4586 \qquad \text{Eq. 8}$$

FP: amount of fine soil particles < 6.3 µm

The second component F_R represents an aggregation of the impacts from soil temperature and soil moisture in relation to optimal conditions and can only be estimated because of the annual time steps in the model. Here is assumed that this factor is aggregated within the annual BAT sum of the tilled system:

$$F_R = \frac{BAT_t}{365}$$ Eq. 9

If the top soil is annually mixed by ploughing all three assumed soil layers have the same weight G_t=1 in the turnover process.
For no-plough conditions, if the soil layers are not mixed, the (virtual) three top soil layers take part in the turnover with the weight values of 1, $1/\alpha$ and $1/\alpha^2$.
This leads to the relation between the BAT values of a tilled (BAT_t) and a non-tilled (BAT_{nt}) system:

$$BAT_{nt} = \frac{BAT_t}{3} \cdot (1 + \frac{1}{\alpha} + \frac{1}{\alpha^2})$$ Eq. 10

3.4 Soil organic matter turnover

3.4.1 Turnover of carbon

Soil organic matter (SOM) dynamics may be handled by different approaches. The CCB approach uses conceptual pools and describes C and N dynamics as well. As the SOM pools in the CCB model have conceptual character they are not measurable (Figure 34).

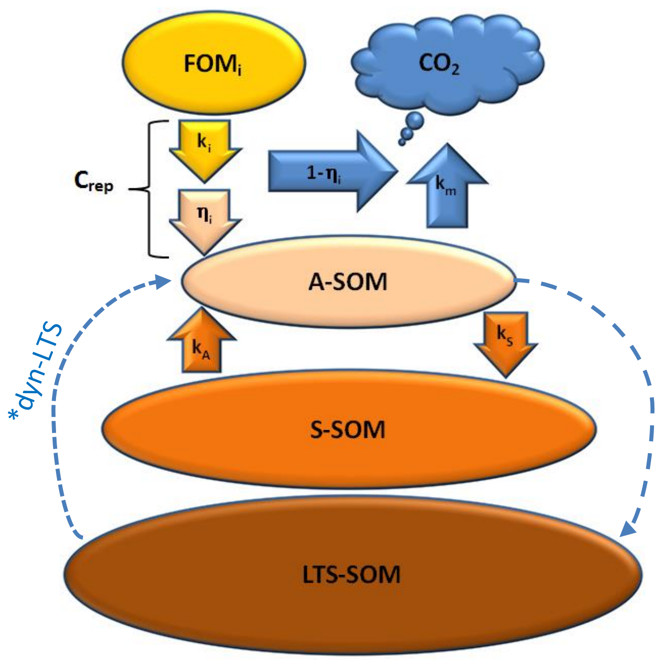


Figure 34: Conceptual pools and fluxes within the soil organic matter module in CCB; *dyn-LTS: only when dynamic LTS-pool is enabled

Organic matter in soil is subdivided into four compartments: (1) fresh organic matter (FOM), (2) biological active soil organic matter (A-SOM), (3) stabilized soil organic matter (S-SOM) and (4) long term stabilized soil organic matter (LTS-SOM). After each time step the resulting pool size for C_{org} can be recalculated from the sum from all SOM pools.

$$C_{org} = C_A + C_S + C_{LTS} \qquad \text{Eq. 11}$$

C_x: carbon content of corresponding compartments of organic matter in soil (C_A = A-SOM, C_S = S-SOM, C_{LTS} = LTS-SOM, C_{FOM} = FOM) in kg C ha-1

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}:

$$\frac{dC_{FOM}(t)}{dt} = \dot{C}_{FOM} = k_{FOM} \cdot C_{FOM}(t) \qquad \text{Eq. 12}$$

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

$$\frac{dC_{rep}(t)}{dt} = \dot{C}_{rep} = \dot{C}_{FOM} \cdot \eta_{FOM} \qquad \text{Eq. 13}$$

The turnover of the active SOM pool includes the reproduction flux from FOM (C_{rep}), the mineralization to CO_2 (turnover 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}:

$$\frac{dC_A(t)}{dt} = \dot{C}_A = \dot{C}_{rep} + k_a \cdot C_S(t) - k_s \cdot C_A(t) - k_m \cdot C_A(t) \qquad \text{Eq. 14}$$

Consequently the carbon turnover of the stable SOM pool is:

$$\frac{dC_S(t)}{dt} = \dot{C}_S = k_s \cdot C_A(t) - k_a \cdot C_S(t) \qquad \text{Eq. 15}$$

Table 3: CCB input variables that pertain to the turnover of carbon

Variable	Definition	Unit	Name in database	Database table
k_{FOM}	Turnover coefficient for the decomposition of fresh organic matter	-	K	cdyopspa
η_{FOM}	FOM synthesis coefficient determining the relation between the production of A-SOM to the FOM decay (=CO_2 production)	-	ETA	cdyopspa

3.4.2 Nitrogen fluxes

Nitrogen fluxes modelled by CCB are closely connected to the carbon turnover. The CCB model considers only the N fluxes but not the mineral nitrogen pool itself hypothesizing an unlimited availability of mineral nitrogen in case of nitrogen immobilization (mineral nitrogen is not limiting the OM turnover). In order to provide information about nitrogen mineralization CCB must be able to describe the interaction between SOM turnover and nitrogen fluxes connected with the turnover of the FOM pools and the mineralisation of the active SOM.

The decomposition of FOM also results in a release of mineral nitrogen controlled by the C/N ratio of the given FOM pool γ_{FOM}:

$$\frac{dN_{FOM}(t)}{dt} = \dot{N}_{FOM} = \dot{C}_{FOM} \cdot \frac{1}{\gamma_{FOM}} \qquad \text{Eq. 16}$$

The FOM decomposition results in the creation of A-SOM. The quantity of nitrogen required for the newly-formed amount of active SOM depends on the C_{rep} flux and the C/N ratio of the active SOM (γ_A=8.5):

$$\frac{dN_{rep}(t)}{dt} = \dot{N}_{rep} = \dot{C}_{rep} \cdot \frac{1}{\gamma_A} \qquad \text{Eq. 17}$$

The turnover of the active SOM pool also includes the mineralization of A-SOM to CO_2. Hypothesizing that nitrogen mineralisation from SOM is controlled by the dynamics of carbon turnover the nitrogen release from the mineralization process is determined by the C/N ratio of the active SOM (k_m = 0.00556 d^{-1}):

$$\frac{dN_A(t)}{dt} = \dot{N}_A = k_m \cdot C_A(t) \cdot \frac{1}{\gamma_A} \qquad \text{Eq. 18}$$

The total nitrogen flux into (positive values) or from (negative values) the pool of mineral nitrogen (N_m) results from Eq. 16, Eq. 17 and Eq. 18:

$$\frac{dN_m(t)}{dt} = \dot{N}_m = \dot{N}_A + \dot{N}_{FOM} - \dot{N}_{rep} \qquad \text{Eq. 19}$$

For better illustration of the nitrogen flux calculations in CCB Figure 35 is presenting two examples with respect to FOM decomposition (N_{FOM}) and nitrogen flux from FOM into A-SOM (N_{rep}). Depending on the C/N ratio of the given FOM pool γ_{FOM} (10 or 20) the FOM decomposition results in a net N mineralization (+2) or immobilization (-3). A possible mineralization of the A-SOM pool is not considered within this example.

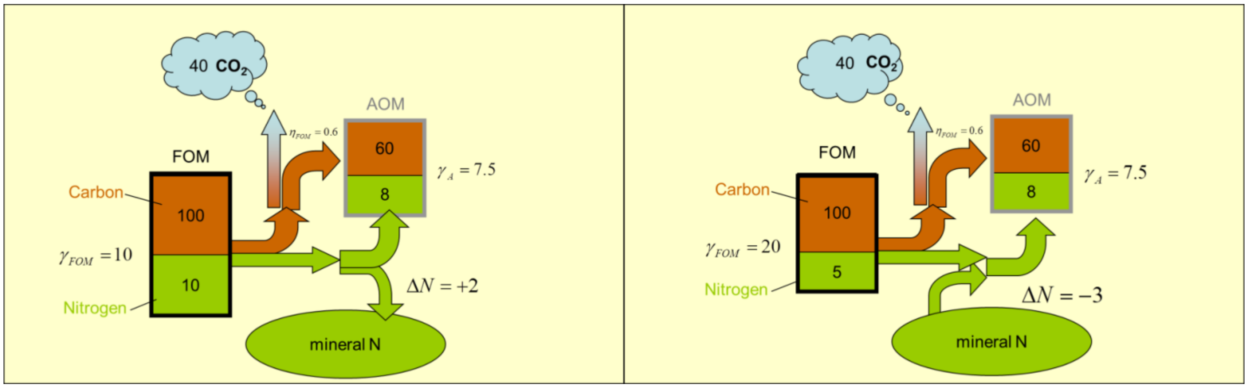


Figure 35: Examples for Net N mineralization and immobilization.

Table 4: CCB input variables that pertain to nitrogen fluxes

Variable	Definition	Unit	Name in database	Database table
γ_{FOM}	C/N ratio of the given FOM pool (substrate specific)	-	CNR	cdyopspa

3.4.3 Soil carbon initialization

At runtime the actual sizes for the active, passive and long term stabilised pool must be initialized. This is based on a given value for C_{org} and N_{org} at t=0. The CCB model will use the values from the measurement data that are indicated with year number 0. Generally it is not recommended to take the first real observation value for this purpose because all observation values include an error and selecting one special observation as initial value would give this result more importance compared to the later observations and the error of the initial value would have an impact on the model results for the following years.

Therefore we recommend to estimate a "virtual" initial value at time t=0 by means of optimisation that gives the model the best fit to the whole set of observations. The sum of squared deviation can be used as a criterion for a good fit and can be minimised by a selection of an optimal initial value leaving all other parameters constant.

A practical implementation of this procedure is available with the OPTIMIZER (http://www.ufz.de/index.php?en=39727) that can be easily connected with CCB and is using the Downhill Simplex Method in multi dimensions as described in detail by Press et al. (1989).

The following paragraph describes the initialization algorithm in more detail:

The carbon amounts of active (C_A) and stabile (C_S) SOM together form the decomposable carbon C_{dec}. The initial value of C_{dec} is the difference between C_{org} and C_{LTS} with an upper limit of 2 M% C_{org}:

$$C_{dec}(0) = MIN\left[2, C_{org}(0) - C_{LTS}(0)\right] \quad \text{Eq. 20}$$

The quantification of C_{LTS} is derived from the CIPS model (Kuka et al., 2007) as proposed by Puhlmann et al. (2006). The amount of carbon stored in soil pores related to the permanent wilting point (*PWP*) is expressed by the factor F_{LTS} and is regarded here as stabilized in the long term:

$$C_{LTS}(0) = C_{org}(0) \cdot F_{LTS} \qquad \text{Eq. 21}$$

with

$$F_{LTS-SOM} = \frac{r_2 \cdot r_3 \cdot PWP}{r_1 \cdot r_2 \cdot PV + r_3 \cdot PWP \cdot (r_2 - r_1) + r_1 \cdot FC \cdot (r_3 - r_2)} \qquad \text{Eq. 22}$$

r_i:	pore radius: r_1=5 µm; r_2=10 µm (soil type “L”: 12 µm); r_3= 500 µm
PWP:	soil moisture at permanent wilting point in VOL%
FC:	soil moisture at field capacity in VOL%
PV:	soil pore volume in VOL%

The amount of $C_{dec}(0)$ is distributed between C_A and C_S according to the model equations (Eq. 23, Eq. 24) assuming steady state conditions.

$$C_A(0) = C_{dec}(0) \cdot \frac{k_a}{k_a + k_s} \qquad \text{Eq. 23}$$

$$C_S(0) = C_{dec}(0) - C_A(0) \qquad \text{Eq. 24}$$

The C/N ratio of the decomposable SOM is fixed to 8.5. If an initial value for $N_{org}(0)$ is known it is used to calculate the C/N ratio of the LTS pool (γ_{LTS}) from the C/N ratio of the complete SOM (γ_{SOM}).

$$\gamma_{LTS}(t) = \frac{8.5 \cdot \gamma_{SOM}(0) \cdot C_{LTS}}{8.5 \cdot C_{org}(0) - \gamma_{SOM}(0) \cdot C_{dec}(t)} \qquad \text{Eq. 25}$$

3.4.4 Dynamics of the physically stabilized SOM

Following the ideas of the CIPS model (Kuka et al., 2007) there is a highly stabilized SOC pool that is associated with the micro pores in soil. Hitherto CCB and CANDY addressed this pool as long term stabilized (LTS-SOM) and assume this pool as constant because changes of this pool size were expected to be insignificant small.

Assuming the LTS-SOM dynamic is controlled by soil physics, the pool size calculation is ruled by following equations:

$$SOC = \alpha \cdot (A_\mu + A_m + A_M) \qquad \text{Eq. 26}$$

α:	areal specific carbon concentration
A:	inner area of micro (µ), meso (m) and macro (M) pores in soil

$$C_{LTS} = \alpha \cdot A_{\mu} \quad \text{Eq. 27}$$

$$C_{LTS} = SOC \cdot \frac{A_{\mu}}{A_{\mu} + A_m + A_M} = SOC \cdot F_{LTS} \quad \text{Eq. 28}$$

F_{LTS}: soil structure depending factor relating the LTS pool size to total SOC

Further details of F_{LTS} calculations were given by Kuka et al. (2007), Puhlmann et al. (2006) and Franko et al. (2011).
In our approach a change of the LTS pool size will be triggered by a change of the wilting point (Θ_{μ}) pore volume that is related via the (virtual) radius *r* and the total length *l* to the inner area of micro pores, assuming cylindrical pores (please also see section '3.5 Estimation of soil parameters'):

$$V_{\mu} = \Theta_{\mu} = \pi \cdot r_{\mu}^2 \cdot l_{\mu} \quad \text{Eq. 29}$$

$$A_{\mu} = 2 \cdot \pi \cdot r_{\mu} \cdot l_{\mu} = 2 \cdot \frac{\Theta_{\mu}}{r_{\mu}} \quad \text{Eq. 30}$$

$$C_{LTS} = 2 \cdot \alpha \cdot \frac{\Theta_{\mu}}{r_{\mu}} = \beta \cdot \Theta_{\mu} \quad \text{Eq. 31}$$

β: variable factor relating the LTS C to the Volume of micro pores

$$\Delta C_{LTS} = \beta \cdot \Delta\Theta_{\mu} \quad \text{Eq. 32}$$

The initial value of β in Eq. 32 is given by

$$\beta = \frac{SOC \cdot F_{LTS}}{\Theta_{\mu}} \quad \text{Eq. 33}$$

This model extension has been applied successfully by Franko and Merbach (2017) to model SOM dynamics on a bare fallow experiment.

Implementation of carbon and nitrogen fluxes

In the CIPS model 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 CCB model behaves very similar to soil microbial biomass. Therefore we assume that the flux between timestep t_i and t_{i+1} to/from the LTS pool is affecting the A-SOM pool and hypothesize that:

$$\Delta C_{LTS} = -\Delta C_A = C_{LTS}(t_{i+1}) - C_{LTS}(t_i) \qquad \text{Eq. 34}$$

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 has to be considered:

$$N_{flx} = \Delta C_A \cdot \frac{\gamma_A - \gamma_{LTS}}{\gamma_A \cdot \gamma_{LTS}} \qquad \text{Eq. 35}$$

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 immobilized during the decomposition of fresh organic matter). A decreasing LTS-SOM pool leads to nitrogen immobilization due to the A-SOM growth and has to be considered as N-sink.

3.5 Estimation of soil parameters

The minimum soil dataset required by the model was limited to clay content (< 2 µm) and soil type (soil textural class) according to the German classification system "Reichsbodenschätzung" (Arbeitsgruppe Boden, 2005; BMJ, 2007; Capelle et al., 2006; Lieberoth, 1982). This requires a number of soil data conversions carried out by pedotransfer functions. If the silt content is known it is not necessary to specify the soil type.

If the content of silt is unknown it is calculated from the German soil classification scheme assuming the mean silt content of the given soil class.

Further the fine (≤ 6.3 µm) and medium (6.3 – 20 µm) silt content is calculated using a loglinear interpolation according to Nemes et al. (1999) between clay and silt.

Interpolation of soil texture

$$p(d_x) = p(d_1) + (\ln(d_x) - \ln(d_1)) \cdot \frac{p(d_2) - p(d_1)}{\ln(d_2) - \ln(d_1)} \qquad \text{Eq. 36}$$

d_i: diameter of particle class

$p(d_i)$: cumulative amount of particles with $d \le d_i$

Soil bulk density

It is possible to calculate soil bulk density using Eq. 37 and Eq. 38 following the approach of standardized bulk density TRD_s (Ruehlmann and Körschens, 2009) to find an appropriate b value.

$$TRD = TRD_s e^{-b \cdot C_{org}} \qquad \text{Eq. 37}$$

$$TRD_s = 2.684 + 140.943 \cdot b \qquad \text{Eq. 38}$$

Following the results of Rühlmann and Körschens (2009) we can express the standardized bulk density as a function of soil clay content:

$$TRD_s = 1.78345 - 0.0081 \cdot clay \qquad \text{Eq. 39}$$

The combination of the last both equations leads to an approach to get b from clay content:

$$b = (1.78345 - 2.684 - 0.0081 \cdot clay)/140.943 \qquad \text{Eq. 40}$$

$$b = -0.00639 - 5.747 \cdot 10^{-5} \cdot clay \qquad \text{Eq. 41}$$

Soil particle density

The particle density (ρ_p) is required in order to calculate the pore volume (*PV*). An useful equation for this purpose was published by Rühlmann et al. (2006):

$$\rho_p = \frac{1}{\frac{Q_{om}}{\rho_{om}} + \frac{1 - Q_{om}}{\rho_m}} \qquad \text{Eq. 42}$$

ρ_{m}: density of mineral component in g cm^{-3}

ρ_{om}: density of organic matter component in g cm^{-3}

where

$$\rho_m = 2.659 + 0.003 \cdot clay \qquad \text{Eq. 43}$$

and

$$\rho_{om} = 1.127 + 0.373 \cdot Q_{om} \quad \text{with} \quad Q_{om} = \frac{C_{org}}{55} \qquad \text{Eq. 44}$$

Hydrological properties

The combination of bulk density and particle density provides the pore volume of the soil:

$$PV = (1 - \frac{\rho_b}{\rho_p}) \cdot 100 \qquad \text{Eq. 45}$$

PV: pore volume in VOL%

In the standard approach (with constant soil physical properties) the values of field capacity (Eq. 46) and permanent wilting point (Eq. 47) are calculated from soil texture using the pedotransfer function published by Lieberoth (1982).

$$FC = 3.40 + 0.85 \cdot ABT \qquad \text{Eq. 46}$$

FC: field capacity in VOL%

ABT: settleable components less than < 10 µm

$$PWP = 1.23 + 0.74 \cdot clay \qquad \text{Eq. 47}$$

PWP: moisture at permanent wilting point in VOL%

The characteristic values *PV*, *FC* and *PWP* of a specific water retention curve are required to calculate the amount of long-term stabilised carbon with the F_{LTS} parameter.

For the simulation of dynamic soil physical properties a more complex approach is used in order to reflect the impact of SOC and BD on hydrological parameters. Generally, the widely used model of Van Genuchten (1980) can be used to predict soil moisture at characteristic matric potential (h=50000 hPa (pF=4.7) for PWP and h=63 hPa (pF=1.8) for FC)

$$\Theta(\Psi) = \Theta_r + \frac{\Theta_s - \Theta_r}{(1 + (\alpha \cdot |\Psi|)^n)^m} \qquad \text{Eq. 48}$$

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]

The parameters of the van Genuchten model are calculated with another pedotransfer function from Vereecken et al. (1989), which calculates the van Genuchten parameters using USDA7 texture classes.

$$\Theta_s = 0.81 - 0.283 \cdot BD + 0.001 \cdot T \qquad \text{Eq. 49}$$

$$\Theta_r = 0.015 - 0.005 \cdot T + 0.014 \cdot C_{org} \qquad \text{Eq. 50}$$

$$\alpha = e^{(-2.486+0.025 \cdot S-0.351 \cdot C_{org}-2.617 \cdot BD-0.023 \cdot T)}T \qquad \text{Eq. 51}$$

$$n = e^{(0.053-0.009 \cdot S-0.013 \cdot T+0.00015 \cdot S^2)} \qquad \text{Eq. 52}$$

$$m = 1 \qquad \text{Eq. 53}$$

3.6 Benchmarks

Benchmarks for a successful evaluation of carbon turnover models have not been established yet. However, one could expect to have values of RMSE, $RMSE_{rel}$, ME, ME_{rel}, SEM and the value of (1-r) as close to 0 as possible.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(O_i - P_i)^2}{n}} \qquad \text{Eq. 54}$$

$$RMSE_{rel} = \frac{100}{\bar{O}} \cdot \sqrt{\frac{\sum_{i=1}^{n}(O_i - P_i)^2}{n}} \qquad \text{Eq. 55}$$

$$ME = \frac{\sum_{i=1}^{i=n}(O_i - P_i)}{n} \qquad \text{Eq. 56}$$

$$ME_{rel} = \frac{100}{\bar{O}} \cdot \frac{\sum_{i=1}^{i=n}(O_i - P_i)}{n} \qquad \text{Eq. 57}$$

$$EF = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O}_i)^2} \qquad \text{Eq. 58}$$

$$SEM = \sqrt{\frac{\sigma^2}{n}} \qquad \text{Eq. 59}$$

$$r = \frac{\sum O_i \cdot P_i - \frac{1}{n} \cdot (\sum O_i) \cdot (\sum P_i)}{\sqrt{\left[\sum O_i^2 - \frac{1}{n} \cdot (\sum O_i)^2\right] \cdot \left[\sum P_i^2 - \frac{1}{n} \cdot (\sum P_i)^2\right]}} \qquad \text{Eq. 60}$$

O_i:	observed value at time step i	M%
P_i:	predicted value at time step i	M%
N:	number of measurements	-
RMSE, $RMSE_{rel}$:	root mean square error	M% or %
ME, ME_{rel}:	mean error	M% or %
SEM:	standard error of the mean difference	M%
Σ:	standard deviation of the difference O-P	M%
r:	Pearson correlation coefficient	-

The correlation between O_i and P_i is significant if the value T_0 (Eq. 61) is not lower than the right-tail value of the Student's t-distribution (p=0.95, f=n-2):

$$T_0(r) = |r| \cdot \frac{\sqrt{n-2}}{\sqrt{1-r^2}} \qquad \text{Eq. 61}$$

Statistical measures of model performance have serious limitations as the different datasets show a considerable heterogeneity in terms of their data quality. Graphical displays can be useful for showing trends, types of errors and distribution patterns. In this study the comparison of observed and predicted values in diagrams was also regarded to judge the quality of model performance at specific sites.

For a comparative evaluation of a CCB calibration with other approaches Akaike's Information Criterion should be calculated in its standard form:

$$AIC = 2 \cdot k + n \cdot ln\left(\frac{\sum(O_i - P_i)^2}{n}\right) \qquad \text{Eq. 62}$$

Or using the corrected version for finite sample sizes:

$$AICc = 2 \cdot k + n \cdot ln\left(\frac{\sum(O_i - P_i)^2}{n}\right) + \frac{2 \cdot k \cdot (k+1)}{n-k-1} \qquad \text{Eq. 63}$$

4 Input-/Output Parameters & Database

4.1 User-data tables

4.1.1 field_description

Content:

Basic information as fixed data with general description of each homogenous simulation object.

attribute	meaning	unit/type
FI_id	Unique identifier	number
Herkunft	Data source / project (documentation purpose)	string
soil_id	pointer to soil data (soilproperties)	number
climate_id	pointer to climate (climate_station → climate_data)	number
Location	Appears as folder name	string
site_description	Appears as plot name	string
comment	Space for remarks	string
versuch_code	Pointer to table experiments	number
area	Plot area	number
I_con	Type of initial condition (obsval, null, pre managment)	string
notill	Selected tillage option (0 for allways, 1 for never, 2 for manual input	string
Mw_bat	Average BAT (updated by the model)	[d a^{-1}]

Remarks:

Depending on the purpose of the model application it is recommended to extend the table to store additional information that may be useful for the result interpretation.

4.1.2 climate_station

Content:

Basic information about the location of the climate station and N-deposition.

attribute	meaning	unit/type
climate_id	Unique identifier	number
station	Name of the site	string
breite	Latitude (documentation purpose)	number
laenge	Longitude (documentation purpose)	number
year0_nd	Initial year for calculated N deposition	Number
year1_nd	Last year for calculated N deposition	Number
ndep_0	N deposition rate of the initial year	Kg/ha
ndep_1	N deposition rate of the last year	number

4.1.3 climate_data

Content:

Climate data in annual time steps.

attribute	meaning	unit/type
climate_id	Pointer to climate_station	number
year	Observation year; a 0 indicates a long term average	number
temperature	Average annual air temperature at 2 m	[°C]
precipitation	Annual precipitation sum	[mm]

Remarks:

Day and month are options for future development and now should be given a 0 value.

4.1.4 cultivation

Content:

Management data.

attribute	meaning	unit/type
cultivation_ID	Unique number	number
FL_ID	Pointer to field description	number
FL_ID_alt	Internal buffer	number
year	Year of activity	number
Macode	Action code; Pointer to cdy_action	number
Item_IX	Object code; pointer to parameter table	number
Sim_Quantity	Internal buffer	number
Quantity	Amount or yield	number
part	Spatial weight (in %), only available in 'regional-mode'	number

Remarks:

Day and month are options for future development and now should be given a 0 value

4.1.5 measurements

Content:

Observed data and initial data for SOC and N_t.

attribute	meaning	unit/type
meas_ID	Unique number	number
FL_ID	Pointer to field_description	number
M_IX	Property code; pointer to cnd_mwml	number
year	Year of observation	number
year_number	Count of the year; 0 means initial value	number
meas_value	Object code; pointer to parameter table	number
Corg_m	Internal buffer	number
vrnz	Varianz of observed value (optional)	number

Remarks:

Day and month are options for future development and now should be given a 0 value.

M_IX=7 : SOC; M_IX=0 : NT

4.1.6 soilproperties

Content:

Parameters of the (top) soil.

attribute	meaning	unit/type
soil_ID	Unique identifier	number
profile	Name shown in the interface	string
BA_RBS	Soil type according to “Reichsbodenschätzung”	string
clay	Clay content [%]	number
silt	Silt content [%]	number
silt_org	y(es) if provided by user	y/n
sand	Sand content [%]	number
sand_org	y(es) if provided by user	y/n
FAT	Fine particles (clay + fine silt) content [%]	number
FAT_org	y(es) if provided by user	y/n
PWP	Permanent wilting point	number
PWP_org	y(es) if provided by user	y/n
PV	Pore volume	number
PV_org	y(es) if provided by user	y/n
FC	Field capacity	number
FC_org	y(es) if provided by user	y/n
PD	Particle density	number
PD_org	y(es) if provided by user	y/n
BD	Bulk density	number

BD_org	y(es) if provided by user	y/n
cif	Part of LTS carbon	number
cif_org	y(es) if provided by user	y/n
skelett	Stone content [%]	number
fbio	Calibration factor for microbial biomass	number

Remarks:

More attributes may be added for convenience of a study.

4.1.7 experiments

Content:

Register of the folder objects (experiments, farms etc.) within the database.

attribute	meaning	unit/type
location	Folder name shown in interface	string
vcode	Unique code	string
exp_id	Unique number	number
herkunft	Description of data origin	string
select	Informal field	number

Remarks:

Don't forget do add a record here if you are manually extending the database.

4.1.8 site_state

Content:

Formal register of the plot objects within the database - only these objects can be selected for simulation.

attribute	meaning	unit/type
FL_ID	Link to field_description	numeric
status	Use for simulation: 1 = use; 0 = skip	numeric
res_val	Informal field	numeric

Remarks:

Don't forget do add a record here if you are manually extending the database.

4.2 Model-parameter tables

Only a selection of the model-parameter tables is described within this CCB-manual. For further information please also see the CANDY-manuals.

4.2.1 CDYAKTION

Content:

Description of management actions.

attribute	meaning	unit/type
ACTION	Name of action	string
ACTION_ID	Key	integer
UNIT_INTENSITY	Unit of the quantitative attribute	string
DEF_INTENSITY	Definition of the quantitative attribute	string

4.2.2 cdyopspa

Content:

Parameters for fresh organic matter turnover.

attribute	meaning	unit/type
item_ix	Index	integer
Name	Name	string
K	Decomposition coefficient	[d^{-1}]
ETA	Synthesis coefficient	number
CNR_ALT	Total C/N-ratio C_{org} / (N_{org} + N_{min})	number
CNR	Ratio in organic matter (C_{org} / N_{org})	number
TS_GEHALT	Dry matter content	[M. %]
C_GEH_TS	C content in dry matter	[M. %]
MOR	Ratio of mineral and organic nitrogen N_{min} / N_{org}	number

4.2.3 cdypflan

Content: Parameters for crops.

attribute	meaning	unit/type
ITEM_IX	Key	integer
NAME	Name	string
ewr_ix	Pointer to a record in cdyopspa to characterise harvest residues and roots	integer
grd_ix	Pointer to a record in cdyopspa to characterise aboveground biomass after ploughing up (not supported in CCB)	integer
kop_ix	Pointer to a record in cdyopspa to characterise by-products	integer
FEWR	factor between N in harvest residues, roots and yield	[kg kg^{-1}]
CEWR	N amount in harvest residues independent from yield	[kg N ha^{-1}]
N_GEHALT	N-concentration in yield	[kg N dt^{-1}]
TS_BEZUG_HP	Dry matter content	
HI	Harvest index	[cm]

4.3 Result tables

For further information on the result tables please see the sections '2.4.4 Results' (esp. regarding error statistics and N-balance tables) and '2.5.2 Checking results'.

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