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Notat i projektet "Få styr på kulstoffet i jorden" – opdatering af C-TOOL modellen

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AU-AGROs specifikke formål i nærværende projekt er at arbejde med opdateringer af inputmodellen (allometriske funktioner) på baggrund af nyeste forsøgsresultater og videnskabelig litteratur, samt med parametriseringen af selve C-TOOL modellen. Der har været afholdt et møde i projektet d. 17. august 2023, hvor ovenstående blev diskuteret.

Mødet samt efterfølgende arbejde har resulteret i følgende notat, som giver en status på det igangværende arbejde med at opdatere C-TOOL modellen.

`rCTOOL`
An open and comprehensive R package for C turnover modelling

Introduction

C-TOOL is widely used valuable model for simulating soil organic matter (SOM) turnover (Petersen et al., 2002; Taghizadeh-Toosi et al., 2014). Its simplicity and flexibility make it a competitive alternative to more complex models that often require extensive input data specific to the intended scenario (Andrén & Kätterer, 1997; Coleman & Jenkinson, 1996; Jensen et al., 1997). C-TOOL has been successfully implemented in Denmark for various research and policy applications (Nielsen et al., 2021; Taghizadeh-Toosi & Olesen, 2016). Recent studies have emphasized the importance of simpler models like C-TOOL in forecasting soil carbon dynamics, particularly due to their ease of application and interpretation of results (Guenet et al., 2022). Moreover, C-TOOL holds potential as a teaching tool for understanding carbon fluxes in agricultural systems.

However, the current implementation of C-TOOL lacks openness, user-friendliness, and comprehensive documentation. Its source code is not publicly available, written in C#, and lacks proper licensing information. The interface is simple but lacks functionality for running multiple scenarios efficiently. Creating inputs for the model is time-consuming and prone to errors. Moreover, there is an absence of guidance for output analysis, hindering understanding and interpretation of the results.

To address these limitations, we have been working on developing an open-source R package, rCTOOL, that encapsulates the capabilities of C-TOOL while addressing its implementation limitations. The aim consists of providing a user-friendly interface, facilitates running multiple scenarios, and offers comprehensive documentation and licensing information. This package streamlines the use of C-TOOL, making it more accessible and effective for potential users.

This transition to the R programming language will expand the user base and provide a platform for continuous improvement and contributions. The R implementation should be built using a basic and streamlined approach, minimizing the reliance on external dependencies. A similar initiative has been successfully demonstrated with the SoilR package (Sierra et al., 2012), which offers an R implementation of the RothC model (Coleman & Jenkinson, 1996). This widely adopted package has been recommended for estimating potential carbon sequestration by the Food and Agriculture Organization (FAO) (Peralta et al., 2022). This experience strongly supports the idea of developing the C-TOOL model as an R package (Wickham & Bryan, 2023). Once the translation is completed, a comprehensive evaluation of the programmed workflow in R is crucial. This evaluation should encompass testing, validation, and verification to ensure that the model functions as intended and produces reliable results.

ADDRESSING THE AMBIGUITIES IN THE CALCULATION CODE

During the translation process from C# to R, we encountered several inconsistencies that stemmed from the transition to an open-source coding language. To address these inconsistencies, we actively collaborated with a colleague at SEGES Innovation P/S, Henrik Vestergaard Poulsen, who provided valuable insights and assistance in resolving or clarifying the identified issues in the actual code and parameter settings.

The following items have been addressed in the new implementation:

Time Step of the Model

The original C-TOOL model had a flexible time step, but later versions were fixed to a monthly time step. However, there seems to be a consensus on using an annual time step for consistency with other models and data sources. Currently, the available codes run on a monthly time step, and the difference in output time scales is solely in how the results are presented. Version 2.3 reports "annual" stocks based on the estimated value for December of each year, while the last version reports the stocks monthly. The time step for the model is now in rCTOOL fixed as monthly, as it aligns with the input data and parameter settings that operate at the same temporal scale. Switching to a monthly basis eliminates the need for the Runge-Kutta equation, which was used to differentiate through time. Consequently, we have removed this element from the code.

Soil temperature Function

We have observed discrepancies regarding the soil temperature function (Equation 3, Annex) and its impact on the temperature factor that influences decomposition rates. The soil temperature function should consider monthly daily average temperatures and monthly daily average ranges. However, the current code only calculates monthly averages and annual ranges. To address this inconsistency, we have modified the code to incorporate monthly temperature ranges and allow the Thermal diffusivity coefficient (k'), affecting the damping depth (D, depth where the soil temperature reaches the maximum) to vary according to the soil type by default. For Danish soil types, reference can be found in Schjønning (2021) and additional pedometric functions can be used following Arkhangelskaya and Lukyashchenko (2018).

Soil temperature function following McCulloch and Penman (1956) through Montien and Unsworth (1994):

$$T_{(z,t)} = \overline{T} + A(0)\exp\left(-\frac{z}{D}\right)\sin\left(\omega t - \frac{z}{D}\right)$$

where $\overline{T}$ is the average monthly air temperature (°C),

$A(0)$ is the average monthly day amplitude in air temperature at the soil surface (°C),

D is the damping depth (m)

$$D = \sqrt{(2 \times k'/\omega)}$$

At the same time: ω is angular frequency of the harmonic oscillation in temperature for (2π/P; P is period it means the length of each cycle, or distance from one peak to the next in this case daily),

k' is the thermal diffusivity coefficient (m^2/day).

In essence the function is the same, but the units and time steps were put in agreement.

Monthly distribution of Carbon Inputs

The documentation and code implementation differ in how the carbon inputs (from plants and amended C) are distributed throughout the year. Annual amended C or extra C divided by 12 and distributed homogeneously in the month added to the topsoil FOM; Manure C inputs assumed to be implemented in month 3 March to the FOM in topsoil FOM and HUM according the humification fraction; C inputs from plants assumed fixed in the months April, May, June and July distributing the annual calculation with the weights 0.08, 0.12, 0.16 and 0.64, respectively. Therefore, now this distribution of the C inputs from plants and the Manure to soil can be defined by the user and the Annual amended C was removed.

Fraction of input going to humified organic matter

Previously, the fraction of manure inputs was added to the topsoil FOM and HUM pools based on a humified fraction that was influenced by the clay content of the soil. This clay dependence has been removed, and it is now indicated that this fraction is determined according to the type of organic fertilization, i.e., the origin of the manure.

Transport to the subsoil

A portion of each C pool in the topsoil is vertically transferred to its corresponding pool in the subsoil. In previous versions, there was inconsistency in the stage of decomposition at which this transport fraction was applied. In the current version, we have modified this approach and now apply the transport fraction to the C in the pool after decomposition. This ensures that the decomposed C can either be respired or complexify into a more stable pool (see the updated Flow chart).

CLAY CONTENT

The model now allows to vary the clay content in top and subsoil. It is relevant to note that this is only affecting the humification fraction applied to the decomposed FOM.

INITIAL POOL SIZE DISTRIBUTION

We have established that the initial pool size distribution, which determines the proportion of C in each pool, should be defined as an input to the model. Any modifications to this initial partitioning should be made before and outside the core functions of the turnover model. This specifically applies to the function that modifies the partitioning based on the C/N ratio, ensuring that the ROM partitioning is increased at the expense of the HUM partitioning.

Updated model explanation

Input variables and parameters

Environmental conditions:

Monthly temperatures:

- Tran (*C) Monthly daily average range temperature
- Tave (*C) Monthly daily average temperature

C inputs:

From plants:

- $\mathrm{Cinput_{top}}$ (Mg/ha*year)
- $\mathrm{Cinput_{sub}}$ (Mg/ha*year). Now derived from allometric.

From manure:

- $\mathrm{Cinput_{man}}$ (Mg/ha*year) Obtained by C proportion in manure type.

Soil:

Clay content: fraction for both horizons

- $\mathrm{clay_{top}}$,
- $\mathrm{clay_{sub}}$

Carbon content initial (Mg/ha) Cinit

Decomposition rates: OM decomposition rates (Mg/month)

- $kFOM$, 0.12
- $kHUM$, 0.028
- $kROM$, 3.858e-05

Transport fraction after decomposition that is assumed to be transported from topsoil to subsoil in each pool: ft is considered constant to 0.003

Initial pool size distribution (proportion can be modified by C/N content or use a default parametrization)

- **CN**, Carbon Nitrogen Relation
- $\mathrm{fFOM} + \mathrm{fHUM}, \ + \mathrm{fROM} = 1$

$$Top\text{: } 0.0316; 0.4803; 0.4881 \; Sub\text{: } 0.003; 0.3123; 0.6847$$

Monthly distribution of C inputs

plant=c(0,0,0,8,12,16,64,0,0,0,0,0)/100

manure=c(0,0,100,0,0,0,0,0,0,0,0,0)/100

Thermal diffusivity coefficient Phi: 0.035

Constant:

- Respiration fraction $\mathrm{f_{CO}}$: 0.62
- Proportion of C in topsoil Cproptop=0.47
- $\mathrm{f_{man}}$ Fraction of manure humified dependent on the type of material (0.12)

- f_{ROMI} "Romification" Fraction

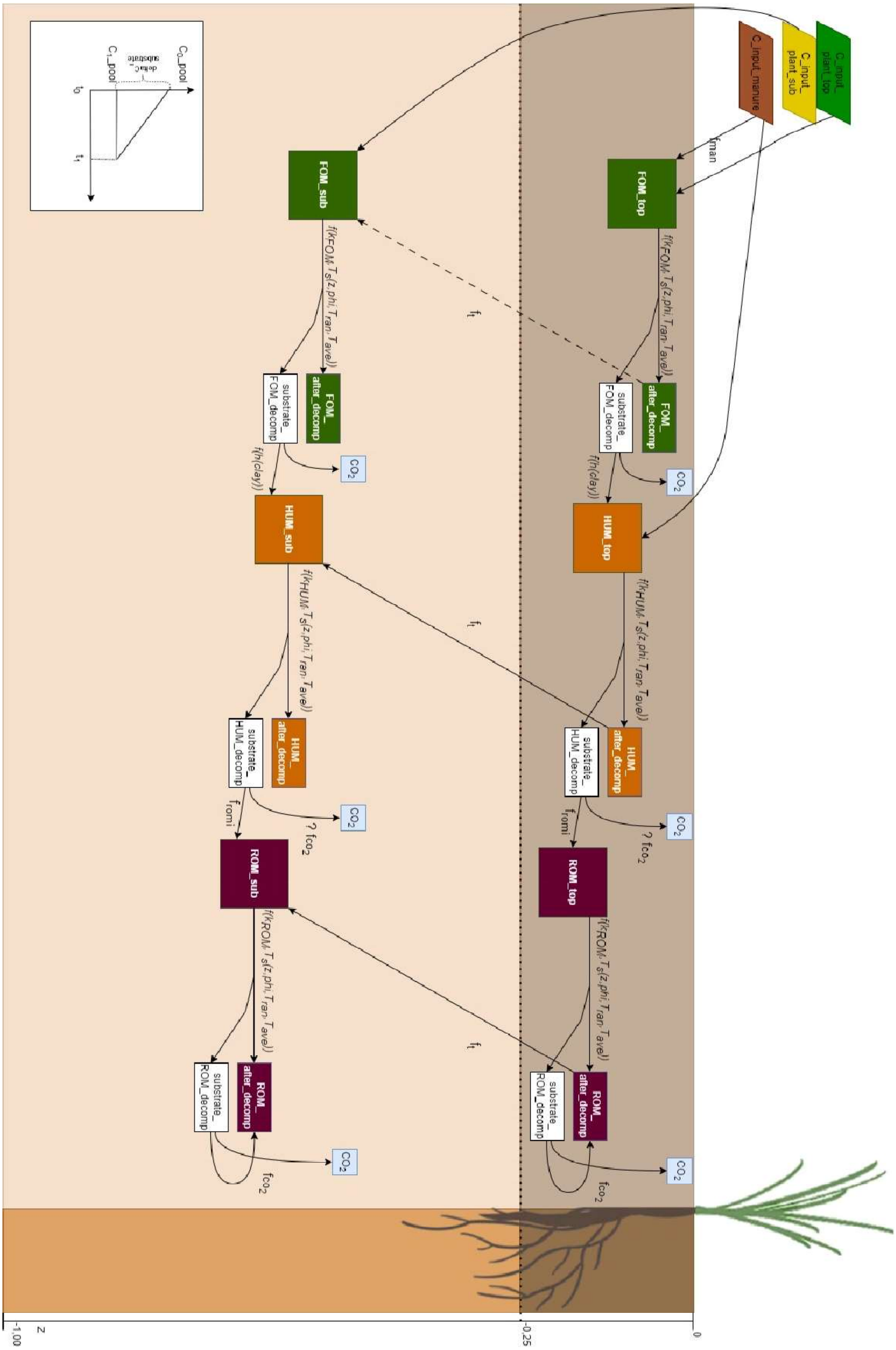
CODING REPOSITORIES

The coding work of the package still in process and can be found in:

https://github.com/francagiannini/ctoolstole.git ;
https://github.com/francagiannini/rCTOOL

CHARTFLOW

We have been working on a chart flow as a conceptual and coding foundation:



Further and ongoing works

Systematic review for Improving C input estimations:

To enhance the accuracy of C-TOOL, a systematic review of the C input estimations is crucial. By improving the estimation methods, we can refine the inputs required to run and calibrate the model effectively. We are now working on a systematic review for a metanalysis manuscript to have an estimation of “Carbon inputs to soil from common agricultural crops in NW Europe”.

Focus on the most important crops under Danish conditions (“NyMarkmodel” project, WP4.2). The crops: Spring barley, Winter wheat, Grass-clover, Silage maize, Winter oilseed rape, Winter rye, Winter barley, Grass for seed, Spring oat, Grass, Potatoes, Sugar beets, Spring wheat, Triticale.

Conceptual framework remaining question

Recalibration

By utilizing long-term experimental data and the enhanced estimation of C inputs, we can undertake a recalibration process. This recalibration will fine-tune the model's parameters and improve its accuracy in simulating real-world scenarios.

Developing different user interfaces and implementations

Having the core code in R we can enhance its usability, adaptability, and accessibility, making it a valuable tool for various users and stakeholders, including researchers, practitioners, and farmers. We need to maintain the classical common approach allowing to organize the inputs in a designated folder, where each input file can be generated using supporting software such as Excel or R. But also build an alternative to feed the model with multidimensional matrices, incorporating parameters related to lag time and soil-scenario parametrization. This design is particularly useful for implementing C-TOOL at a national or regional scale, utilizing information derived from GIS. To support this, the preprocessing outputs should include spatiotemporal visualization and descriptions to aid in data interpretation. Finally, it would be nice to have a user-friendly Interface to make C-TOOL accessible to a wide range of users for playing. This interface should allow anyone to propose a scenario, test it, and obtain processed outputs in the form of figures and tables. We can easily make this trough shiny app (Chang et al., 2017; Chang et al., 2015) and hosted in a website (see gallery of examples) maintained by the university ensures availability and ease of access.

Annex

Previous documentation

To maintain a record of the previous work related to the development and implementation of the C-TOOL model, below is compiled a list of the reviewed documentation. Please note that this list does not include theses and conference presentations.

C-TOOL Documentation	
Article	Type
Petersen, B. M., Olesen, J. E., & Heidmann, T. (2002). A flexible tool for simulation of soil carbon turnover. *Ecological modelling*, *151*(1), 1-14. **https://doi.org/10.1016/S0304-3800(02)00034-0**	Model development
Petersen, B. M. (2003). C-TOOL version 1.1. A tool for simulation of soil carbon turnover. Description and users guide. **Internal file**	Model description / User guide
Petersen, B. M., Berntsen, J., Hansen, S., & Jensen, L. S. (2005). CN-SIM—a model for the turnover of soil organic matter. I. Long-term carbon and radiocarbon development. Soil Biology and Biochemistry, 37(2), 359-374. **https://doi.org/10.1016/j.soilbio.2004.08.006**	Related / Model framework
Petersen, B. M., (2010). *A model for the carbon dynamics in agricultural, mineral soil.* AGRO Department Aarhus University. **Internal file**	Model description / Application
Kemanian, A. R., & Stöckle, C. O. (2010). C-Farm: A simple model to evaluate the carbon balance of soil profiles. European Journal of Agronomy, 32(1), 22-29. **https://doi.org/10.1016/j.eja.2009.08.003**	Application
Petersen, B. M., Knudsen, M. T., Hermansen, J. E., & Halberg, N. (2013). An approach to include soil carbon changes in life cycle assessments. *Journal of Cleaner Production*, *52*, 217-224. **https://doi.org/10.1016/j.jclepro.2013.03.007**	Application
Taghizadeh-Toosi, A., Christensen, B. T., Hutchings, N. J., Vejlin, J., Kätterer, T., Glendining, M., & Olesen, J. E. (2014). C-TOOL: A simple model for simulating whole-profile carbon storage in temperate agricultural soils. *Ecological Modelling*, *292*, 11-25. **https://doi.org/10.1016/j.ecolmodel.2014.08.016**	Model development/ calibration
Taghizadeh-Toosi, A. (2015). C-TOOL. **Institutional web**	Model description / User guide
Taghizadeh-Toosi, A., Christensen, B. T., Glendining, M., & Olesen, J. E. (2016). Consolidating soil carbon turnover models by improved estimates of belowground carbon input. *Scientific Reports*, *6*(1), 32568. **https://www.nature.com/articles/srep32568**	Application
Keel, S. G., Leifeld, J., Mayer, J., Taghizadeh-Toosi, A., & Olesen, J. E. (2017). Large uncertainty in soil carbon modelling related to method of calculation of plant carbon	Application

input in agricultural systems. European Journal of Soil Science, 68(6), 953-963. **https://doi.org/10.1111/ejss.12454**	
Taghizadeh-Toosi, A., & Olesen, J. E. (2016). Modelling soil organic carbon in Danish agricultural soils suggests low potential for future carbon sequestration. Agricultural Systems, 145, 83-89. **https://doi.org/10.1016/j.agsy.2016.03.004**	Application
Riggers, C., Poeplau, C., Don, A., Bamminger, C., Höper, H., & Dechow, R. (2019). Multi-model ensemble improved the prediction of trends in soil organic carbon stocks in German croplands. Geoderma, 345, 17-30. **https://doi.org/10.1016/j.geoderma.2019.03.014**	Application
Hu, T., Taghizadeh-Toosi, A., Olesen, J. E., Jensen, M. L., Sørensen, P., & Christensen, B. T. (2019). Converting temperate long-term arable land into semi-natural grassland: decadal-scale changes in topsoil C, N, 13C and 15N contents. European Journal of Soil Science, 70(2), 350-360. **https://doi.org/10.1111/ejss.12738**	Application
Taghizadeh-Toosi, A., Cong, W. F., Eriksen, J., Mayer, J., Olesen, J. E., Keel, S. G., ... & Christensen, B. T. (2020). Visiting dark sides of model simulation of carbon stocks in European temperate agricultural soils: allometric function and model initialization. Plant and Soil, 450, 255-272. **https://doi.org/10.1007/s11104-020-04500-9**	Application
Taghizadeh-Toosi, A., & Christensen, B. T. (2021). Filling gaps in models simulating carbon storage in agricultural soils: the role of cereal stubbles. Scientific Reports, 11(1), 18299. **https://doi.org/10.1038/s41598-021-97744-z**	Application
Hansen, J. H., Hamelin, L., Taghizadeh-Toosi, A., Olesen, J. E., & Wenzel, H. (2020). Agricultural residues bioenergy potential that sustain soil carbon depends on energy conversion pathways. *GCB Bioenergy*, *12*(11), 1002-1013. **https://doi.org/10.1111/gcbb.12733**	Application
Farina, R., Sándor, R., Abdalla, M., Álvaro-Fuentes, J., Bechini, L., Bolinder, M. A., ... & Bellocchi, G. (2021). Ensemble modelling, uncertainty and robust predictions of organic carbon in long-term bare-fallow soils. Global Change Biology, 27(4), 904-928. **https://doi.org/10.1111/gcb.15441**	Application
Gasser, A. A., Diel, J., Nielsen, K., Mewes, P., Engels, C., & Franko, U. (2022). A model ensemble approach to determine the humus building efficiency of organic amendments in incubation experiments. Soil Use and Management, 38(1), 179-190. **https://doi.org/10.1111/sum.12699**	Application

Coding background

Based on the available documentation and AU Foulum internal documents, the primary individuals involved in code development were Bjørn Molt Petersen and later Jonas Vejlin, along with Arezoo Taghizadeh-Toosi. Bjørn Molt Petersen was initially responsible for developing versions 1.0 and 1.1 (CN-SIM) in C++, while working in or in relation to the department until 2010. It appears that version

1.0 has been the basis for subsequent developments. During 2014 and 2015, Jonas Vejlin and Arezoo Taghizadeh-Toosi contributed to the project by creating a C# version, which was also programmed in MATLAB. This period gave rise to the last compiled version found, ctool2.3, which is accompanied by the main documentation available on the website (Taghizadeh-Toosi, A. (2015). C-TOOL. Institutional web). Thereafter, a later code, referred to as *CtoolStandalone*, was developed, which can be considered an improvement in terms of code readability. This code is what we consider the last version.

C-TOOL

Model

(Adapted from last documentation (Taghizadeh-Toosi, 2015))

C-TOOL considers the inputs and turnover of C associated with three SOC pools in the topsoil (25 cm depth) and three corresponding pools in the subsoil (from 25 to 100 cm depth), the transport of SOC from topsoil to subsoil, and emissions of CO_2. Simulation of ^{14}C natural abundance is also facilitated.

The input soil variables are clay content, soil temperature, soil C/N ratio, and the type and quantity of organic matter inputs.

The turnover of C in each pool is described by first-order reaction kinetics:

EQUATION 1

$$\frac{dC_i}{dt} = -k_i C_i F_T(T)$$

where k_i is decomposition rate coefficient (yr^{-1}) for pool i at standard temperature conditions define as 10 °C, C_i is the C content in pool i (Mg C ha^{-1}) and $F_T(T)$ is the temperature coefficient that is modified to obtain unity at 10 °C according to Kirschbaum (1995), as following:

EQUATION 2

$$F_T(T) = 7.24\, exp\left(-3.432 + 0.168T\left(1 - \frac{0.5T}{36.9}\right)\right)$$

where T is temperature (°C).

The depth (z) and time (t) variability of soil temperature is described using the function of Monteith and Unsworth (2013):

EQUATION 3

$$T_{(z,t)} = \overline{T} + A(0)\exp\left(-\frac{z}{D}\right)\sin\left(\omega t - \frac{z}{D}\right)$$

where $\overline{T}$ is the average monthly air temperature (°C), $A(0)$ is the monthly amplitude in air temperature at the soil surface (°C), D is the damping depth (m), and ω is angular frequency of the harmonic oscillation in temperature, 2π/P; P is period (the length of each cycle, or distance from one peak to the next). The turnover is simulated in monthly bases using a Runge-Kutta method to resolve the estimation of the decay rate affected by temperature in Equation 1.

After simulating the turnover of FOM, a proportion (t_F) of the C is allocated to the subsoil, and the remaining C undergoes humification. Here, the clay content influences the humification coefficient

(h), which is the proportion of C that is partitioned to the HUM pool. The clay response function is from:

EQUATION 4

$$R = 1.67(1.85 + 1.6\, exp(-7.86\, X))$$

where R is the ratio $(C\ lost\ as\ CO_2)/(C\ directed\ to\ HUM)$, and X is clay fraction in the soil (kg kg^{-1}). Usually, a constant of 1.67 is used to adjust to observed values of R (Coleman and Jenkinson, 1996). The humification coefficient (h) is then calculated as:

EQUATION 5

$$h = \frac{1}{R} + 1$$

Note that with this equation, the humification coefficient ranges from 0.148 in soil without clay to 0.244 in a hypothetical situation of a soil with 100 % clay. The amount of SOC that is removed either by transport to the subsoil or emitted as CO_2 from the HUM pool is calculated simultaneously after the decomposition process. The same procedure is applied to the ROM pool. (proportion of SOC initially present as ROM depends on the history of the soil (Thomsen et al., 2008).)

In C-TOOL, the C/N ratio is used to partition SOC between the HUM and ROM pools, using the function:

EQUATION 6

$$f(cn) = min(56.2cn - 1.69, 1)$$

where cn is the C/N ratio. This function returns a value less than one when the C/N ratio is above a threshold value of 10.8. This threshold was determined from an independent dataset of Danish agricultural soils (Thomsen et al., 2008).

With respect to vertical transport of SOC, C-TOOL model uses a one-way, convection type transport model for simulating vertical transport of C in the soil (Jenkinson and Coleman, 2008). This model represents a simplification of the transport patterns reported in previous studies (Bruun et al., 2007; Dörr and Münnich, 1989). In C-TOOL, the transport of C occurs from all topsoil pools (0–25 cm depth) to the corresponding subsoil pool (25–100 cm). Then, for the subsoil pools, the vertical transport of SOC is also calculated but the amount of SOC is brought back to the donating SOC pool.

Feeding the model

The model itself needs information about:

- Average monthly mean air temperature (˚C),
- Soil initial condition:
  - Clay content (as a proportion),
  - Initial soil C/N ratio,
  - Initial fraction pool distribution (FOM, ROM and HUM) for topsoil and subsoil
- C inputs
  - Yearly C inputs of plant residues (Mg C ha^{-1}) in topsoil
  - Yearly C inputs of plant residues (Mg C ha^{-1}) in subsoil

Yearly C inputs from organic fertilization trough manure.

Carbon inputs

Dimensioning C inputs coming from plants implies implementing allometric relationships with crop yields. For cereals, dry matter yield was reported separately for grain and straw, whereas for other crops, only total above-ground biomass was reported. It is known that even when straw is harvested, there will be C inputs going back to the soil (Jørgensen et al. 2007). For example, the belowground C inputs from dead root biomass and rhizodeposition as well as the stubble (Berntsen et al. 2005). Many frameworks to estimate C inputs of topsoil and subsoil can be used for each crop. Nevertheless, in C-TOOL usually the allometric functions implemented has been descripted by (Taghizadeh-Toosi et al., 2014):

Parameters

α = Harvest index of main crop product relative to aboveground biomass

β = Root biomass and exudate C (below-ground C) as proportion of total net C assimilation

δ = Biomass of secondary crop product (e.g. straw) as proportion of yield of main crop product

ζ = Proportion of secondary crop product that is harvested

ε = Concentration of C in biomass DM (kg Mg^{-1})

ξ = Proportion of root and exudate C deposited in top soil (0-25cm)

Input

Y_{main} = DM yield of main crop product (Mg DM ha^{-1})

C partitioning

C_{main} = C yield of main crop product $= \varepsilon Y_{main}$

C_{tot} = total C assimilation $= 1/((1 - \beta)\ \alpha)\ C_{main}$

The above-ground carbon in crop residues (C_{resid}) is calculated as:

If there is only one crop product or if the secondary product is not harvested:

$$C_{resid} = (1/\alpha - 1)\ C_{main}$$

If the secondary product is harvested:

$$C_{resid} = (1/\alpha - 1 - \delta\ \zeta)\ C_{main}$$

The below-ground carbon in root residues and exudates (C_{resid}) are calculated as:

$$C_{below} = \beta\ C_{tot} = \beta\ /((1 - \beta)\ \alpha)\ C_{main}$$

The C in residues, roots and exudates deposited in topsoil ($C_{rootTop}$) is calculated as

$$C_{rootTop} = C_{resid} + \xi\ C_{below}$$

The C in residues, roots and exudates deposited in subsoil ($C_{rootSub}$) is calculated as

$$C_{rootSub} = (1 - \xi)\ C_{below}$$

Actual implementation utilizing the executable ctool2.3

C-TOOL runs in C++ compiled application that is file-driven executed through a file named ctool2.3.exe. Executing, by clicking on it or by any terminal command, the app will search a file (*runscenarios.txt*) where is specified the location path of the input's files needed. The inputs files needed are:

- Temperature file <- .txt file with the monthly mean temperatures of the entire simulation period (including initialization)
- Data file <- .txt file with the yearly C Inputs in topsoil, subsoil and as manure fertilizer
- Input file <- .txt file with all the parameters corresponding to soil, initial soil C situation and decomposition rates for each pool

- Mode<- .txt file with a “0” character

An R code is now available to build these files, call and execute the app and finally read and summarize the outputs.

sim_building code makes allometric calculation and defines input file parameters and save it in a table called *tbl_fill which* is a table where each row is a scenario and each column a parameter. Based on *tbl_fill* parameters *make_data* code runs by row (by scenario) generating a list: *aver*

aver is a list of lists in which each element contains: - the id - the data table - and the input file. For each element in *aver run_ctool* code makes a folder and runs C-TOOL on it.

Finally, *outputs* code reeds the outputs in each folder and copy it to a single finale data table where the observational unit is the combination of year and the scenario (the scenario provides as multiple dimensions as combination in the simulation design has been made)

CTOOL conceptual framework limitations

The simplicity of the model carries many advantages, but it is evident that it also represents some limitations that should be stated explicitly. It is crucial to note that the model does not consider soil water as a limiting factor when simulating C turnover over decades, assuming that temperature is the overarching climatic driver for C turnover in the European temperate area from which data for parameterization was retrieved. The model is therefore not applicable to soils exposed to prolonged dry seasons and neither under excessively wet conditions that with low redox potentials may be restricting SOM degradation. Nevertheless, an indirect effect on Soil moisture dynamic can be now incorporated by modifying the C inputs calculation. Also, C-TOOL does not consider the effects of soil tillage intensity nor bulk density changes during the simulation period that can be affecting C sequestration process (Six et al., 1998; Six et al., 2000).

C-TOOL as most SOC models rely on C input data from harvest residues or decaying plant parts (above- and belowground) and organic amendments. The plant C inputs are derived from measured agricultural yields using simple allometric equations that establish the relation between C inputs and crop yields (Keel et al., 2017). Different published approaches of estimating C input have been compared leading to the conclusion that there are still large uncertainties in simulated changes in SOC (Keel et al., 2017). Other aspect is that the evidence of this allometric relations and the sources of variability has been mostly studied for crops leading a mayor uncertainty on grasslands behavior and other cultivated species (Smith et al., 2020; Taghizadeh-Toosi & Christensen, 2021). Moreover, there is sufficient evidence to believe that the C inputs from plants belowground biomass are not a function of aboveground biomass behavior and that may be a smarter decision to rather use a fixed amount for each specific crop under specific conditions (Hirte et al., 2018; (Jacobs et al., 2020); Taghizadeh-Toosi and Christensen, 2021).

Another question that always emerge working with pool distributed models is about initialization period and the initial pool size distribution to get a steady state equilibrium of pools necessary to evaluate SOC storage (Taghizadeh-Toosi et al., 2020; Xu et al., 2011). Particularly C-TOOL consists of three pools Fresh Organic Matter (FOM, half-life of 0.5 year), Humified Organic Matter (HUM, half-life of 20 years), and Resistant Organic Matter (ROM, half-life of 1500 years). Even though good model performance has been achieved in external validation based on long-term experimental data, the impact of modifying the initial distribution of SOC among these pools in the model remains unclear (Taghizadeh-Toosi et al., 2020). In general terms the parametrization chosen for C-TOOL implementations has been done based on experimental experience with no effort in testing any distributional approach considering parameters as random variables or any error propagation which limits the possibility of counting with outputs uncertainty measurements.

References

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Andrén, O., & Kätterer, T. (1997). ICBM: the introductory carbon balance model for exploration of soil carbon balances. *Ecological applications*, *7*(4), 1226-1236.

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