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me4soc was developed as part of the <u>HoliSoils</u> project (Holistic management practices, modelling and monitoring for European forest soils, H2020 Grant Agreement No 101000289) to simulate forest soil organic carbon (SOC) stocks and greenhouse gas (GHG) fluxes at site scale. Relevant project deliverables for this webtool are: D 2.1, D2.2, D2.4.

**Title** Multi-model Ensemble interface for Soil Organic Carbon predictions

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**Host server** deployed using Shiny Server and hosted on the institutional server of the Geology Lab of the École Normale Supérieure (ENS), Paris.

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First year available: 2024.

**Software version**: v1.

Size of archive: 11 GB.

Program language: R.

**Software Availability**: http://me4soc.geologie.ens.fr/, CC BY-NC 4.0 licence.

Data Availability: Open for use with any suitable data. All other datasets used come from

open-source databases.



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#### 1. Introduction

The HoliSoils H2020 project aims to advance modelling tools for monitoring soil properties and GHG fluxes. One of the objectives is to develop an interactive interface that launches state-of-the-art models to simulate SOC stocks and GHG fluxes at site scale. The goal of the interactive interface is to allow end-users, i.e., land use, land use change and forestry (LULUCF) experts and scientists, to simulate SOC stocks and GHG fluxes following scenarios of climate, land-use and land management change. This document describes the v1 of the interface, which builds upon the v0 developed as part of deliverable 2.2 and integrates new models, data and features. The interface has a clear and user-friendly structure with a sidebar menu including: a description of the tool, the models used and scenarios built, a section for data input, and one to visualize and download the model outputs. The user is asked to enter the required data to launch the models. If all the data is not available, by specifying the geographical coordinates of the site, the tool is launched with data extracted from global or regional databases in opensource repositories.



#### 2. The online interface

The online interface (v1) of the multi-model ensemble tool was developed using the Shiny app framework (R Core Team, 2022) and is publicly available at the following link: <a href="mailto:me4soc">me4soc</a>.

The website has a clear and user-friendly structure with a sidebar menu including different sections: **Description**, **Data**, **Outputs**, and **About**. In the following paragraphs, we describe each section in detail.

When the geographic coordinates of the site are inserted, the tool automatically extracts soil, litter and climate data from pre-processed regional and global databases (Table 1). That is, the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP) database (Frieler et al., 2017) for climate and litter input data, the European LUCAS database (De Brogniez et al., 2015; Yigini and Panagos, 2016; Ballabio et al., 2016, 2019) for measurements of soil data and derived products, the Plant Trait (TRY) database (Kattge et al., 2020) and Yasso manual (Liski et al., 2009) for species-specific litter chemical properties, and the Global Monitoring Laboratory (GML) database for mean annual global marine atmospheric CH<sub>4</sub> concentration (Lan et al., 2022). This feature allows the models to be run over Europe even if all the required data is not available. However, measured site data should be prioritized, when possible.

Table 1 References and sources of the online opensource repositories used to extract the required data to launch the models.

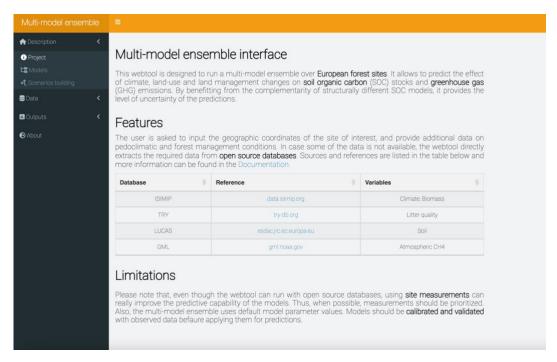
Short-name	Reference	Variables
ISIMIP	(Frieler et al., 2017)	Climate, Biomass
TRY	(Kattge et al., 2020)	Litter quality
LUCAS	(De Brogniez et al., 2015; Yigini and Panagos,	Soil
	2016; Ballabio et al., 2016, 2019)	
GML	(Lan et al., 2022)	Atmospheric CH <sub>4</sub>

#### 2.1 Description

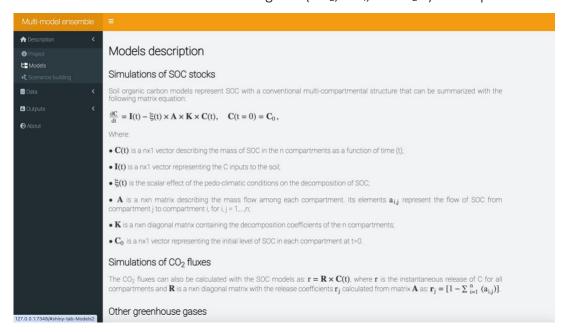
The Description section has three subpanels: **Project, Models,** and **Scenarios building**.

The Project subsection is the homepage of the interface and consists of: an
explanation of the project, the objectives of the multi-model ensemble tool, the data
used from opensource repositories. It also highlights the limitations of the tool to the
user and its domain of applicability.





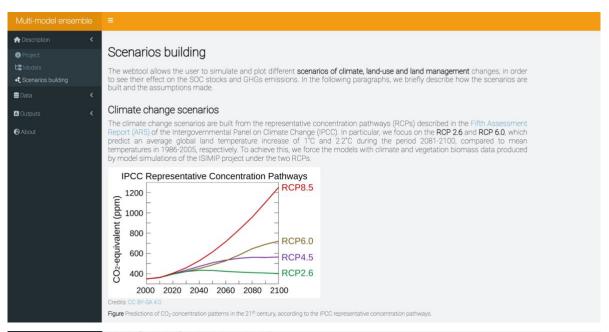
• The **Models** subsection describes the models used for the simulations and provides references for each one of them. A description of the technical procedure used to calculate the SOC stocks and GHG gases (CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O) is also provided.



 The Scenarios building subsection describes in detail the climate, land-use and land management scenarios used in the simulations and provide references and assumptions for each one of them.

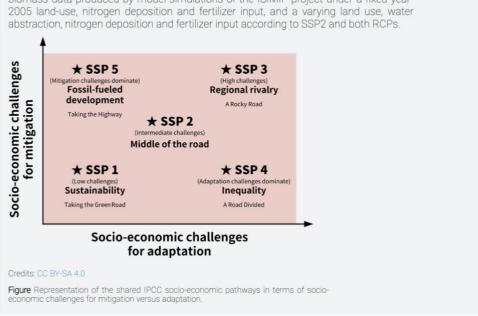




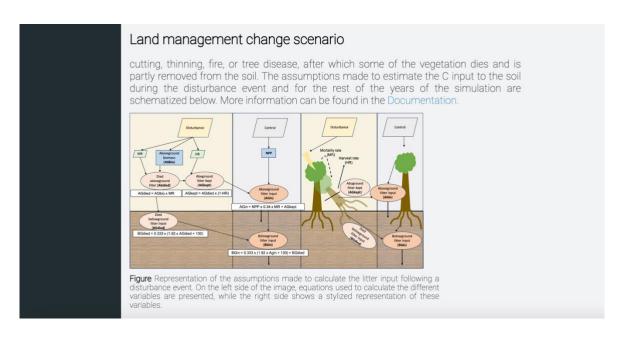


#### Land-use change scenario

The land-use scenarios are derived from the shared socio-economic pathways (SSPs) defined in the IPCC Sixth Assessment Report (AR6). In particular, we focus on the SSP2, which contemplates social, economic and technological trends that do not shift markedly from historical patterns. To achieve this, we force the models with vegetation biomass data produced by model simulations of the ISIMIP project under a fixed year-2005 land-use, nitrogen deposition and fertilizer input, and a varying land use, water abstraction, nitrogen deposition and fertilizer input according to SSP2 and both RCPs.



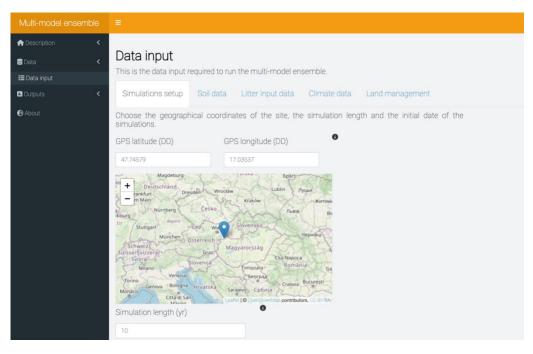




#### 2.2 Data

The Data section has one subpanel called **Data input**.

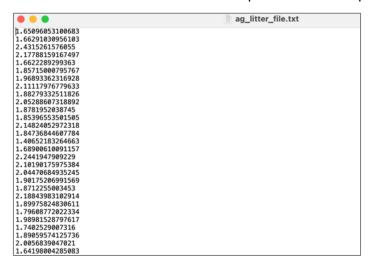
**Data input** is an interactive subsection where the users are asked to input their data. It is subdivided into five parts, separating different data types: **Simulation setup**, **Soil data**, **Litter input data**, **Climate data** and **Land management**. Each variable has a tooltip marked with an "info" icon that describes in detail the information required and the references used for default values.





- The Simulation setup requests the geographic coordinates of the site (latitude and longitude, in decimal degrees), the simulation length (in years), and the starting date of the simulations (YYYY-MM-DD). In this subpanel, it is possible to visualize the chosen location from a map.
- The **Soil Data** section requests soil information of the site. That is, <u>clay</u> and <u>silt</u> concentration (%), <u>SOC stocks</u> (Mg C ha<sup>-1</sup>), <u>soil thickness</u> (cm), <u>C:nitrogen</u> (C:N) ratio, and <u>bulk density</u> (Mg m<sup>-3</sup>).

The **Litter input data** section requests data on the plant inputs. That is, the <u>dominant tree species</u> of the site, which the user can select from a list; the <u>annual aboveground C input</u> to the soil (Mg C ha<sup>-1</sup> yr<sup>-1</sup>), which should be input as a .csv or .txt file, having one column with rows referring to the annual aboveground C input in chronological order, such as in the picture below; the <u>annual belowground C input</u> to the soil (Mg C ha<sup>-1</sup> yr<sup>-1</sup>), input similarly as the annual aboveground C input; the chemical composition of the litter input, that is: <u>acid hydrolysable compound fraction</u>, <u>water soluble compound fraction</u>, <u>ethanol soluble compound fraction</u>, neither soluble nor hydrolysable compound fraction, the <u>lignin:nitrogen ratio</u>, the <u>lignin fraction</u>, and the <u>size of the woody litter</u> (cm). If data is not available, the ISIMIP database will be used for litter input data (see section 4.3.1) and the TRY database for the litter chemical composition of tree species.



The Climate data section requests data on the climate variables. That is, <u>daily</u>
 <u>surface temperature</u> (°C), <u>daily precipitation</u> (mm), <u>monthly potential</u>



evapotranspiration (mm month<sup>-1</sup>), and <u>daily volumetric soil water content</u> (mm mm<sup>-3</sup>) for the simulation time period. This data should be input as a .csv or .txt file, having one column with rows referring to the variable's values in chronological order. The user should also input the <u>average climate data for the decades</u> <u>preceding the simulations</u>. For example, if simulations start on January 2020, this should be the average climate data between 1990 and 2020, or a similar time period. If the user does not dispose of all the required data, then data from the ISIMIP repository will be extracted and the RCP 2.6 data with fixed land-use will be used for the land management scenario simulations (see section 4).

Finally, the <u>atmospheric CH<sub>4</sub> concentration</u> (ppm) at the beginning of the simulations is required. If the data is not available, the global marine annual database (GML) will be used to extract atmospheric CH<sub>4</sub> concentration for the first available data.

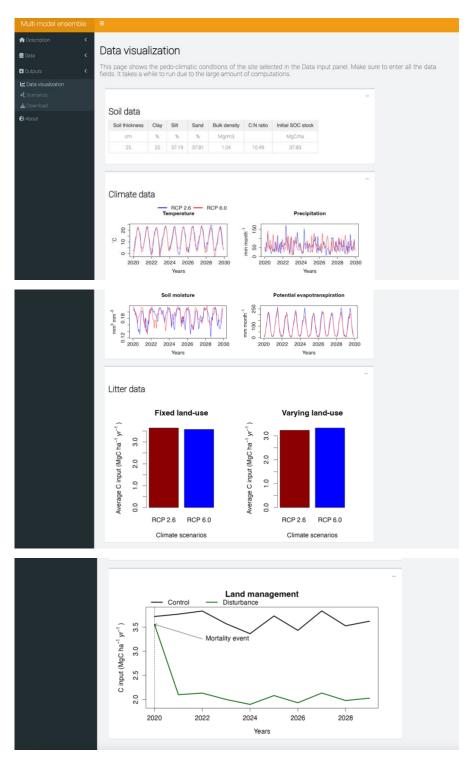
• The Land management section requests data on the disturbance event, such as fire, cutting, thinning, or tree disease. That is, the year of disturbance (number of the year since the beginning of the simulations), the aboveground and belowground biomass before the disturbance event occurred. If no data is available, model outputs of total biomass will be extracted from the ISIMIP database, and the amount of aboveground and belowground biomass will be calculated assuming that they are equal. Finally, the user is asked to insert the rate of mortality (%) of the vegetation, that is the percentage of trees that died after the event, and the harvest rate (%) of the dead aboveground biomass.

#### 2.3 Outputs

The Outputs section has three subpanels: **Data visualization**, **Scenarios**, and **Download**.

 The Data visualization subsection generates tables and graphs from the input variables selected by the user or extracted from opensource databases. That is, soil data, climate data for the different climate scenarios (and from user input, if it is the case), and litter input data for the different land-use and land management scenarios.





• The **Scenarios** subsection shows graphs of the multi-model simulations. In particular, it shows the evolution of SOC stocks and CO<sub>2</sub> fluxes throughout the selected simulation length.

It is divided into three parts: one for **Climate Change**, one for **Land-use Change**, and one for **Land Management** scenarios.



■ The **Climate Change** panel shows simulations of SOC stocks and CO<sub>2</sub> fluxes from the multi-model ensemble forced with RCP 2.6 and RCP 6.0 climate variables, and fixed year-2005 land-use litter input. In this panel, it is possible to modify the clay concentration (%) to see its effect on the simulations, by sliding a bar indicating the current level of clay.



• The Land-use Change panel shows the multi-model ensemble simulations of SOC stocks and CO<sub>2</sub> fluxes under RCP 2.6 and RCP 6.0 climate scenarios, and varying land-use litter input according to SSP2.



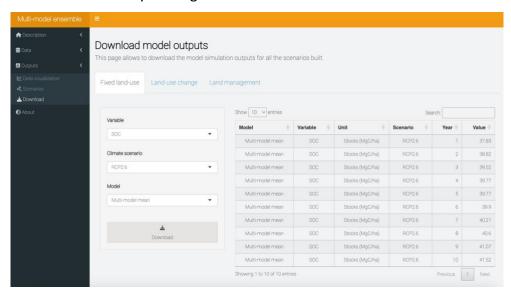
■ The Land Management panel shows the multi-model ensemble simulations of SOC stocks and CO<sub>2</sub> fluxes under the control and disturbed scenario. In this panel, it is possible to modify the mortality rate (%) and harvest rate (%) of the



vegetation, to see how they affect SOC stocks and CO<sub>2</sub> fluxes, compared to the control.



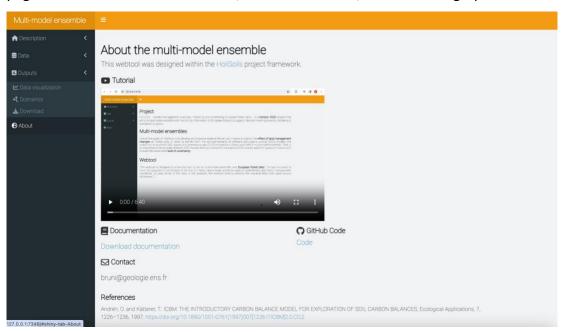
• The Download subsection allows the users to select the model outputs that they wish to download. For each scenario (Climate change, Land-use change, and Land management), the user can: select the variable (SOC, CO<sub>2</sub>, N<sub>2</sub>O, and CH<sub>4</sub>), the model (Multi-model mean, Century, Roth-C, ICBM, Yasso07, Yasso20, SG), and the scenario (RCP 2.6 and RCP 6.0/ control and disturbed), visualize the output data, and download the selected table by clicking on the Download button.





#### 2.4 About

The **About** section provides additional information on the interface. In particular, it provides a link to the HoliSoils website, a tutorial on how to use the multi-model tool (that will be updated once the tool is tested and validated), the documentation of the tool, the GitHub page where all the codes are stored, a contact address, and the bibliographic references used.



### 3. Models

#### 3.1 Simulation of SOC stocks

The v1 of the multi-model ensemble tool includes five SOC models and one empirical model allowing for the estimation of GHG fluxes (CO<sub>2</sub>, N<sub>2</sub>O and CH<sub>4</sub>).

The SOC models represent SOC with a conventional multi-compartmental structure that can be summarized with the following matrix equation:

$$\frac{d\mathbf{C}}{dt} = \mathbf{I}(t) - \xi(t) \times \mathbf{A} \times \mathbf{K} \times \mathbf{C}(t), \mathbf{C}(t=0) = \mathbf{C_0}$$

Where:

- C(t) is a nx1 vector describing the mass of SOC in the n compartments as a function of time (t);
- I(t) is a nx1 vector representing the C inputs to the soil;
- ξ(t) is the scalar effect of the pedo-climatic conditions on the decomposition of SOC;



- **A** is a nxn matrix describing the mass flow among each compartment. Its elements  $a_{i,j}$  represent the flow of SOC from compartment j to compartment i, for i, j = 1, ..., n;
- **K** is a nxn diagonal matrix containing the decomposition coefficients of the n compartments;
- $C_0$  is a nx1 vector representing the initial level of SOC in each compartment at t=0.

The CO<sub>2</sub> fluxes can be calculated from the SOC models as:  $r = \mathbf{R} \times \mathbf{C}(t)$ , with r being the instantaneous release of C for all n compartments, and  $\mathbf{R}$  being a nxn diagonal matrix having the release coefficients  $r_i$  calculated from matrix  $\mathbf{A}$  as:  $r_i = 1 - \sum_{i=1}^{n} (a_{i,i})$ .

Each model differs from one another by the number of compartments, the way and rate at which compartments transfer C within each other, the environmental functions that affect SOC decomposition, and the decomposition coefficients of the compartments (Figure 1). Specific information for each model can be found in their reference paper (Parton et al., 1988 for Century; Coleman and Jenkinson, 1996 for Roth-C; Andrén and Kätterer, 1997 for ICBM; Tuomi et al., 2009 for Yasso07; Viskari et al., 2022 for Yasso20) and in the SoilR package documentation (Sierra et al., 2012).

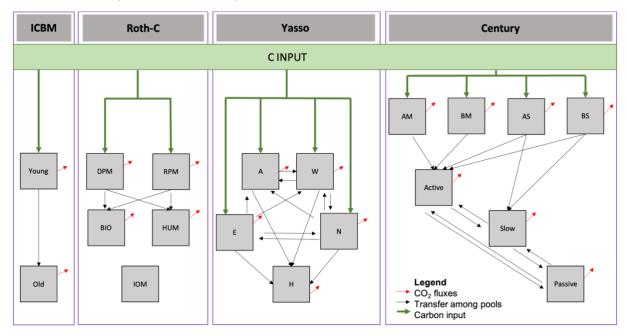


Figure 1 Schematization of the SOC models used in the ensemble. Each box represents a SOC compartment where the C is transferred (black arrows), or respired (red arrows). DPM, RPM BIO, HUM, IOM = decomposable plant material, resistant plant material, microbial biomass, humified organic matter, inert organic matter; AM, BM, AS, BS = aboveground metabolic, belowground metabolic; aboveground structural, and belowground structural.



#### 3.2 Model resolution

To solve the equations of the SOC models, the initial partitioning of C in the different pools needs to be estimated. To do that, we run the models with constant inputs until all the SOC pools reach a steady-state. That is, the annual variation of SOC in all pools is lower than 0.1% for at least 10 years. As forcing, we use the average climate and environmental conditions of the decades preceding the onset of the simulations. In order to match the observed total SOC stocks, we rescale the total simulated SOC using the value of measured SOC provided by the user, and we keep the same estimated proportion of C in each pool as at steady-state (Dimassi et al., 2018). Finally, we solve the matrix differential equation for the specified simulation length. More information on the resolution technique and functions used can be found in the SoilR documentation.

#### 3.3 Simulation of other GHG fluxes

In addition to the CO<sub>2</sub> fluxes, CH<sub>4</sub> uptake and N<sub>2</sub>O fluxes are also estimated using the SG models (Hashimoto et al., 2011). These are simple empirical models allowing to estimate GHG fluxes using data on soil physiochemical properties, water and temperature.

#### 4. Scenarios

The scenarios built for the multi-model ensemble tool allow to simulate climate, land-use and land management changes effects on the SOC stocks and GHG emissions. In the following paragraphs, we briefly describe how the scenarios were built and the assumptions that were made.

#### 4.1 Climate change scenarios

The climate change scenarios are built from the representative concentration pathways (RCPs) described in the Fifth Assessment Report (AR5) of the Intergovernmental Panel on Climate Change (IPCC) (Pachauri et al., 2015). In particular, we focus on the RCP 2.6 and RCP 6.0, which predict an average global land temperature increase of 1°C and 2.2°C during the period 2081-2100, compared to mean temperatures in 1986-2005, respectively. To achieve this, we force the models with climate and vegetation biomass data produced by model simulations of the ISIMIP project under the two RCPs (Frieler et al., 2017). Climate and vegetation variables from



the ISIMIP repository were derived for different models, and averaged. Hence, the forcing variables used in the tool are multi-model averages. The models from which the data were extracted are listed in Table 2 for each climate forcing variable. Daily data was monthly averaged to reduce the data size of the tool.

Table 2 Models of the ISIMIP repository used to estimate the multi-model average climate forcing.

Variable	Climate model	Vegetation model
Daily precipitation (mm)	ipsl-cm5a-lr, miroc5	
Daily temperature (°C)	ipsl-cm5a-lr, miroc5	
Monthly potential evapotranspiration		
(mm month <sup>-1</sup> )	ipsl-cm5a-lr, miroc5	orchidee
Daily soil moisture (m m <sup>-3</sup> ) (top 18 cm)	ipsl-cm5a-lr, miroc5	orchidee

#### 4.2 Land-use change scenario

The land-use scenarios are derived from the shared socio-economic pathways (SSPs) defined in the IPCC Sixth Assessment Report (AR6) (Masson-Delmotte et al., 2021). In particular, we focus on the SSP2, which contemplates social, economic and technological trends that do not shift markedly from historical patterns. To achieve this, we force the models with vegetation biomass data produced by model simulations of the ISIMIP project under a fixed year-2005 land-use, nitrogen deposition and fertilizer input, and a varying land use, water abstraction, nitrogen deposition and fertilizer input according to SSP2 and both RCPs (Frieler et al., 2017). The models from which the data were extracted are listed in Table 3 for each variable. The NPP variable was used to estimate the aboveground and belowground C input (see subsection 4.3).

Table 3 Models of the ISIMIP repository used to estimate the multi-model average C input forcing.

Variable	Climate model	Vegetation model
Net primary production ( $MgC ha^{-1} yr^{-1}$ )	ipsl-cm5a-lr, miroc5	dlem, lpj-guess
Total biomass $(MgC ha^{-1})$	ipsl-cm5a-lr, miroc5	dlem, lpj-guess

#### 4.3 Land management change scenario

The land management scenario is based on user input data. It considers a disturbance event such as cutting, thinning, fire, or tree disease, after which some of the vegetation dies and is partly removed from the soil. The assumptions made to estimate the C input to the soil during



the disturbance event and for the rest of the years of the simulation are schematized in Figure 2.

#### 4.3.1 Control scenario

The aboveground and belowground C input to the soil is either input by the user or calculated from model simulation outputs derived from the ISIMIP repository, protocol 2b (Frieler et al., 2017). Following Malhi et al. (2011), we estimate aboveground litter input from NPP (Neumann et al., 2018) as:

$$AG_{control}(MgC ha^{-1}yr^{-1}) = NPP \times 0.34$$

Where the NPP variable (MgC  $ha^{-1}yr^{-1}$ ) is derived from ISIMIP and averaged across multiple models (Table 3), for both RCP 2.6 and RCP 6.0 scenarios.

Belowground litter input is estimated with the equation from Jonard et al. (2017) as:

$$BG_{control}(\text{MgC ha}^{-1}\text{yr}^{-1}) = 0.333 \times (1.92 \times AG_{control} \times (\text{conversion}_{factor}) + 130)/$$
  
(conversion<sub>factor</sub>)

Where conversion factor is the conversion factor from MgC ha<sup>-1</sup> to gC m<sup>-2</sup>.

#### 4.3.2 Disturbance scenario

We assume that the aboveground C input of the disturbance scenario is equal to:

$$AG_{disturbance} \text{ (MgC ha}^{-1}\text{yr}^{-1}\text{)} = \begin{cases} AG_{control}, & \text{for } t < D \\ AG_{alive}, & \text{for } t > D \\ AG_{alive} + AG_{biomass\;kept}, & \text{for } t = D \end{cases}$$

#### Where:

- D is the year of the disturbance and t is time;
- $AG_{alive} = AG_{control} \times \left(1 \frac{\text{mortality rate}}{100}\right)$  is the aboveground C input from alive vegetation;
- $AG_{biomass\ kept} = AG_{biomass} imes rac{ ext{mortality\ rate}}{100} imes \left(1 rac{ ext{harvest\ rate}}{100}
  ight)$  is the dead aboveground biomass that is kept in the soil, with  $AG_{biomass}$  being either input by the user, or calculate as:  $rac{cveg}{2}$ , cveg being the total vegetation biomass extracted by multimodel simulation outputs from the ISIMIP repository (Table 3).

The belowground C input of the disturbance scenario is then calculated as:



$$BG_{disturbance} \text{ (tC/ha/yr)} = \begin{cases} BG_{control}, & \text{for } t < D \\ BG_{alive}, & \text{for } t > D \\ BG_{alive} + BG_{biomass\ died}, & \text{for } t = D \end{cases}$$

#### Where:

- $BG_{alive} = 0.333 \times (1.92 \times AG_{alive} \times (conversion_{factor}) + 130)/$ (conversion<sub>factor</sub>) is the belowground C input from alive vegetation;
- $BG_{biomass\ died}=0.333 \times (1.92 \times FOL_{died} \times (conversion_{factor}) + 130)/$   $(conversion_{factor})$  is the dead aboveground biomass kept in the soil, with  $FOL_{died}=0.15 \times (AG_{biomass}+BG_{biomass}) \times \frac{mortality\ rate}{100}$  being the dead foliar litter (Konôpka et al., 2021), and  $AG_{biomass}$  and  $BG_{biomass}$  being either input by the user, or their sum being equal to cveg.

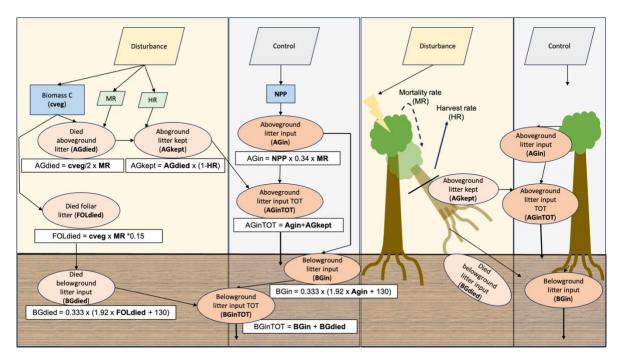


Figure 2 Representation of the assumptions made to calculate the litter input following a disturbance event. On the left side of the image, equations used to calculate the different variables are presented, while the right side shows a stylized representation of these variables.

# 5. Partner and stakeholders' engagement

Partner and stakeholder needs have been considered during the development process of the site. The content has been produced with partner contributions. In particular, we gathered feedbacks from partners of WP2, WP5, WP7, as well as project coordinators.



### 6. Possible further developments

This v1 of the multi-model ensemble interface can currently be launched locally. Because of its large data size, only once tested and validated the application will be deployed online. Moreover, its flexible design allows the tool to be further developed. For example, by including additional models and selecting alternative opensource databases. Including global databases for example, would enable the tool to be applied worldwide. However, the models should be evaluated beforehand to ensure their applicability at the global scale.

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