

First of all, I am happy with the all changes that are made after the first revision. It improved the article! However I still have some remarks.

Thank you very much for your careful comments. We improved the manuscript following the reviewer's suggestions. Details are given below.

First I don't understand the reaction of the authors on reviewer #2:

"Page 10, line 8: Remark. The method of changing one parameter at the time. This is a popular method. However, it renders no information on the effects of interactions of the parameters and that it covers only a limited part of the entire parameter space.

We agree with reviewer #2 that there could be some interactions between sensitivity of different parameters, but testing this was beyond the scope of this study."

My question is: why is performing a good sensitivity analyses beyond the scope of this study? This is a weak reply of the authors on this remark.

Sorry, we failed to clearly explain the challenge of doing what the reviewer is asking. We explored the sensitivity of our model results at three different sites for 8 parameters. Taking a high (+50%) and low (-50%) value for each parameter individually leads to 16 simulations per site, i.e. 48 simulations in total. As changing a parameter's value has a potential impact on the whole carbon dynamic, each simulation required a new spin-up, looping 300 time over the climate forcing.

A full factorial experiment as suggested by the reviewer would need to change up to 8 parameters at the same time. For 8 parameters with 3 possible values each, the number of combination is  $3^8$ , that is 6561 simulations per site, i.e. almost 20,000 simulations in total.

This is well beyond the capability of our computation resources, and hence is not feasible in the framework of this study. Hence we chose to stick with the traditional simple method of changing one parameter at a time.

However, the effect of "interactions of parameters" is a valid point, and in the final manuscript we mention that limitation of our sensitivity analysis:

"We note that our sensitivity analysis, changing one parameter at a time, does not investigate the potential interactions between different parameters."

My second remark is on the following reaction:

"Page 10, line 8: Why 50%? 10 or 5% was also enough to say something about the sensitivity around the default values.

Since the derived model parameters from literature already had their own level of uncertainty, for instance CUE which has more than 50% or K DOC with 5-40% of uncertainty, we took the 50% of change to test all the parameters at the reasonable degree."

Firstly I got the impression that the authors are a little bit confused. An uncertainty range is not needed to perform a sensitivity analyses. To avoid effects of a possible non-linear behaviour of the model, a small range is in general better. Besides this, the authors claim that they took 50% change for all parameters. However table S4 says something different. Also table 1 says something different. For example parameter D<sub>f</sub> has a change of 33%. This table (and also table 2) has also a unit of Kg, which was one of the remarks of reviewer #1.

From the results in figure 8, we show that even with a change in parameter values of +/- 50%, for most parameters, the results hardly change. A 5-10% change in those parameters would lead to virtually no changes in the simulated DOC. Also, our model is essentially linear (see main model's equations in the manuscript, most fluxes follows first order reaction rate), so we are not too worried about larger perturbations. We still believe that changing the parameter values by +/- 50% is a valid choice to clearly show the insensitivity of the model to some parameters, while still exploring possible ranges for these parameters.

Indeed, we did not use the 50% range for the parameter  $D_f$ , as  $D_f$  depends on the soil type, with values ranging between 0.25 (100% clay and/or silt) and 1.0 (100% sand), for slope factor of 0.75 ( see equation 5). It would not make sense to have a slope factor larger than 1.0 in this equation, it would lead to non-physical negative values of  $D_f$  for 100% clay and/or silt. Hence our restricted range for that parameter, going from 0.5 (-33%), to 1.0 (+33%). This is now clarified in the final version of the MS:

"In order to test the sensitivity of DOC related model parameters on the DOC concentration in different depths of the soil profile, simulations were performed with varying values for  $z_0$ ,  $\tau_z$  and DOC controlling parameters such as  $K_{DOC (labile)}$ ,  $K_{DOC (recalcitrant)}$ , slope parameter of  $D_f$ , CUE,  $K_D$  and  $D$  (Table 1).

In total, 16 runs were performed by modifying each parameter once by increasing it 50% and once by decreasing it by 50%, except for the slope parameter controlling  $D_f$  (eq. 5) which was changed by 33% to remain within the physical boundaries."

Kg is corrected to kg.

Other remarks:

Figure 6: Unit Kg is used.

Corrected

Figure 8: This is a representation of information that is given in table S4 and S5. I don't understand this information. Table S4 gives 16 results. I think that set-1 is used to calculate the 'relative change' (how defined?). The second set has a global  $\beta_z$ , but that is not in the figure 8, nor in table S5. But why not change  $z_0$  into two directions? I don't know. Why is  $z_0$  for Carlow coloured red and having a positive relative change? Please make this information consistent with each other.

There was a typo in supplement document:

$\beta_z$  is corrected to  $z_0$ .

As well as in S4 we changed Set-1 from default to PFT based  $z_0$  and Set-2 from global  $\beta_z$  to global  $z_0$ .

Despite all the other sites, Carlow was the only site that using global value of  $z_0$  was giving the positive change. This is now clarified in text:

"In contrast to the other sites, global  $z_0$  leads to a low but still significant positive change of 6.5% in simulated DOC within 3 meters of soil (p-value <0.05, Table S6) (Fig. 8-c)."

Table S1 and S2: Z\_0 instead of z\_0.

Corrected

Figure S3: Unit Kg is used. Which depth is the DOC concentration?

Corrected. Down to 3 m averaged. This is added to revised text.

Figure S4: “-” sign is missing in the unit on the y axis

Corrected

pag 5 supplement: references to figure S4 and S5 are wrong. On pag 7 the references to tables are wrong. Please check all the references to tables and figures!

Corrected

Figure S5: “-” sign is missing in the unit on the y-axis and x-axis.

Corrected

Figure S6: C is missing in the unit on the y-axis.

Corrected

Is the reference at the end still needed?

removed

My advice is that the authors should go through the manuscript to fix the problems and to make the supplementary material consistent with the main text.

# Representation of dissolved organic carbon in the JULES land surface model (vn4.4\_JULES-DOCM)

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**Abstract.** Current global models of the carbon (C) cycle consider only vertical gas exchanges between terrestrial or oceanic reservoirs and the atmosphere, thus not considering lateral transport of carbon from the continents to the oceans. Therefore, those models implicitly consider that all the C which is not respired to the atmosphere is stored on land, hence overestimating the land C sink capability. A model that represents the whole continuum from atmosphere to land and into the

25 ocean would provide better understanding of the Earth's C cycle and hence more reliable historical or future projections. A first and critical step in that direction is to include processes representing production and export of dissolved organic carbon in soils. Here we present an original representation of Dissolved Organic C (DOC) processes in the Joint UK Land Environment Simulator (JULES-DOCM) that integrates a representation of DOC production in terrestrial ecosystems based on incomplete decomposition of organic matter, DOC decomposition within the soil column, and DOC export to the river

30 network via leaching. The model performance is evaluated in five specific sites for which observations of soil DOC concentration are available. Results show that the model is able to reproduce the DOC concentration and controlling processes including leaching to the riverine system which is fundamental for integrating terrestrial and aquatic ecosystems. Future work should include the fate of exported DOC in the river system as well as DIC and POC export from soil.

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## 1 Introduction

An estimated  $1.9 \text{ Pg C yr}^{-1}$  is exported from soils through the river network to the oceans, which represents a significant flux in global carbon (C) cycle (Cole et al. 2007; Regnier et al. 2013) and can affect biological and chemical properties of both aquatic (Aitkenhead & McDowell 2000) and terrestrial ecosystems (Kalbitz 2000). In land surface models that are part of Earth system models, only vertical fluxes of carbon between land and atmosphere are considered whilst lateral export fluxes are not included. This leads to an overestimation of soil organic C (SOC) sequestration and terrestrial C sinks (Janssens et al. 2003; Jackson et al. 2002). Hence we need to move towards a boundless C cycle model which accounts for lateral fluxes and thus produces more accurate projections of atmospheric  $\text{CO}_2$  concentrations and C stocks (Battin et al. 2009). One of the lateral fluxes that has been neglected is the transfer of carbon from terrestrial to aquatic ecosystems in the form of dissolved organic C (DOC), which has been shown to be increased by anthropogenic perturbation such as land use change such as deforestation and increased atmospheric  $\text{CO}_2$  concentrations (Regnier et al. 2013). DOC contributes about 37% of the global riverine carbon exports to the coast (Meybeck 1993) and adds to the net-heterotrophy of inland waters and related  $\text{CO}_2$  emission fluxes to the atmosphere.

The main sources of DOC in terrestrial ecosystems are plant residues (Khomutova et al. 2000), humus and root exudates (Kalbitz et al. 2000; Van den berg et al. 2012; Marschner 1995). DOC within the soil can be the product of in-situ production or be brought in by advective fluxes with soil water transport. It has been hypothesized that loss of the carbon from the soil by leaching has to be taken into account to reasonably re-assess the terrestrial C budget of Europe (Siemens 2003). The fate of this DOC within inland water networks, i.e. the proportion transported to the coast or respired and emitted to the atmosphere, is the key to understanding the link to the other compartments of the Earth system (Cole et al. 2007; Battin et al. 2009). Nevertheless, it is a difficult task to link riverine and terrestrial fluxes by empirical methods, because 1) riverine fluxes are integrating fluxes from different land use systems (Kindler et al. 2011; Boyer & Groffman 1996) with different leaching rates and DOC quality, 2) in-stream transformation makes it difficult to trace back terrestrial DOC sources, and 3) the difficulty to separate natural and anthropogenic perturbation fluxes (Schelker et al. 2013; Regnier et al. 2013).

A physical-based modelling approach explicitly representing different terrestrial sources and processes involved in DOC cycling within the soil column and DOC leaching from the soil can help overcome these difficulties. Representation of DOC cycling within the soil column is also a major step toward simulating deep soil SOC formation (Rumpel & Kögel-Knabner 2011). Physical-based models help to understand the processes involved in soil DOC cycling and leaching as well as biogeochemistry of SOC in general. So far several models have been developed that simulate DOC with different temporal and spatial resolution, from 15 minutes as in SOLVEG-II (Ota et al. 2013) to monthly as in ECOSSE (Smith et al. 2010) or RivCM (Langerwisch et al. 2015) and from site scale as in DyDOC (Michalzik et al. 2003) to global scale as in TEM (Kicklighter et al. 2013). Some of these models represent DOC leaching, whereas others do not. Each model has its own particular definition for carbon pools (including DOC) and DOC production processes which can be based on turnover time, as in TERRAFLUX (Neff & Asner 2001), or based on chemical composition as in the DyDOC model (Michalzik et al.

2003). Although all these models have been evaluated, with the exception of the TEM model which was tested for arctic rivers, none of them has demonstrated its ability of representing the DOC production, processing and transport at the global scale.

In general, most of the models containing decomposition are based on first-order kinetics (Olson 1963). Frequently, models tend to represent the top soil layer as the major source for DOC production and export (Koven et al. 2013), other studies (Rumpel & Kögel-Knabner 2011; Braakhekke et al. 2013) highlight the importance of DOC for SOC production in deeper soil layers.

Here we present an original representation of DOC processes in the Joint UK Land Environment Simulator (JULES-DOCM) that integrates a representation of DOC production in terrestrial ecosystems based on incomplete decomposition of organic matter, DOC decomposition within the soil column, and DOC export to the river network via leaching. JULES has been used to evaluate the global C cycle (e.g. LeQuéré, et al. 2015, Sitch et al. 2015) and its role in the Earth system, but to date lacks the critical processes of DOC production and export. The aim of this study is to include a representation of DOC produced in terrestrial soils down to 3 meters (as soil hydrology and Carbon are simulated over 3 meter soil profile in JULES), assuming an incomplete decomposition of organic matter and its subsequent fate as DOC including i) DOC decomposition and release as CO<sub>2</sub> to the atmosphere, and ii) DOC export to the riverine system via leaching; to test the new model in different ecosystems and to evaluate it against specific sites where soil DOC measurements were available. Other forms of C need different processes to be represented to fully represent the land-to-ocean aquatic continuum of the global C cycle. Hence future work should include DIC and POC export from soils as well as the fate of all exported carbon in the river system.

## **2 Material and Methods**

### **2.1 JULES model**

JULES is a process-based model which represents energy, water and C cycling between vegetation, soil and atmosphere as described in Best et al. (2011) and Clark et al. (2011). Vegetation processes in JULES are represented in a dynamic vegetation model (TRIFFID), distinguishing 9 plant function types (PFTs) at the global scale: tropical and temperate broadleaf evergreen trees, broadleaf deciduous trees, needle-leaf evergreen trees and deciduous trees, C3 and C4 grasses, and evergreen and deciduous shrubs (Harper et al. 2016).

The representation of SOC in JULES, follows the formulation of the RothC soil carbon scheme (Jenkinson et al. 1990; Jenkinson & Coleman 2008), distinguishing four carbon pools: decomposable plant material (DPM), resistant plant material (RPM), heterotrophic microbial biomass (BIO) and long-lived humified material (HUM). DPM and RPM pools receive litter inputs directly from the vegetation due to defoliation, mortality and disturbance, the allocation to DPM or RPM depending on the PFT characteristics with higher fraction of decomposable litter provided from grasses and higher fraction of resistant litter provided from trees (Clark et al. 2011). HUM and BIO each receive inputs from the other two soil carbon pools, as a fraction of the decomposition that is not respired to the atmosphere.

## 2.2 JULES-DOCM model new features

JULES-DOCM is an extension of JULES based on version 4.4 (vn4.4 documentation in <http://jules-lsm.github.io/vn4.4>) , which explicitly represents DOC cycling in soils and considers DOC leaching from the soil profile. The following section deals with the representation of DOC fluxes and processes in more details.

### 2.2.1 Soil carbon profile

SOC is specified as the main source of DOC in JULES-DOCM. In JULES v4.4, each of the four SOC pools is treated as a single box down to 3 m, without any representation of its vertical distribution. This absence of vertical distribution has consequences in terms of simulating DOC fluxes, but also potential impacts on soil CO<sub>2</sub> fluxes, considering vertical variations of soil temperature and moisture. In JULES-DOCM, we introduce a vertical distribution of SOC for each soil carbon pool assuming an exponential decay with depth, with a weighting factor  $\beta_0$  :

$$\beta_{0_i} = e^{-\frac{z_i}{z_0}} \times dz_i \quad (eq.1)$$

Here,  $z_0$  is the e-folding depth of C content within 1 meter of soil (i.e. depth at which SOC decreases by a factor of  $e$  relative to the surface),  $z_i$  is the soil depth of layer  $i$ , and  $dz_i$  is the thickness of the soil layer. In order to estimate  $z_0$ , we used the soil data from Jobbágy & Jackson (2000) that provides the vertical distribution of SOC within a 3 m soil profile based on the observed soil carbon profiles across several biomes. Jobbágy & Jackson provides soil C content in the first meter [0-1m] and for the first 3 meters [0-3m], allowing us to estimate the fraction in the first meter and derive  $z_0$  accordingly:

$$\int_0^1 e^{-\frac{z}{z_0}} dz = x \int_0^3 e^{-\frac{z}{z_0}} dz \quad (eq.2)$$

where  $x$  is the ration of SOC content within the first 1 meter of soil relative to the 3-meter profile for different biomes as given by Jobbágy & Jackson (in their Table. 3) (Jobbágy & Jackson 2000). Jobbágy & Jackson provide data for 11 PFTs. Here we first estimate  $z_0$  for each of those PFTs, then regrouped them into the 9 JULES PFTs (see tables S1 and S2). In order to calculate the fraction of SOC that is used as input for DOC production in each layer of the DOC model, (see equation 4 below) the weighting factors are normalised ( $\beta_{zi}$ ):

$$\beta_{z_i} = \frac{\beta_{0_i}}{\sum_{i=1}^4 \beta_{0_i}} \quad (eq.3)$$

### 2.2.2 DOC fluxes and processes

In JULES-DOCM, four new DOC carbon pools have been added. First the model accounts for a labile and a recalcitrant DOC pool based on their decomposition rate (Aguilar & Thibodeaux 2005; Thibodeaux & Aguilar 2005). The labile pool is readily available for decomposition in soil solution at all times and the recalcitrant pool is subject to slower decomposition rate (Smith et al. 2010). DOC produced from plant material pools (DPM and RPM) and microbial biomass (BIO) is directed to the labile pool, while DOC from humus (HUM) is directed to the recalcitrant pool. Second, both the labile and the recalcitrant DOC pools have a dissolved and an adsorbed form, with only the dissolved pool being subjected to decomposition and leaching.

DOC production ( $F_p$ ) follows first-order kinetics (Olson 1963) and the flux of carbon from SOC to DOC pools ( $k$  for labile or recalcitrant) in each soil layer ( $i$ ) in  $\text{kg C m}^{-2} \text{ day}^{-1}$  ( $F_{p,i}$ ; arrows a-d Fig. 1) is calculated as:

$$F_{p_{k,i}} = \beta_{z_i} \times S_{C_k} \times \left( 1 - e^{(-K_P \times F_S(S)_i \times F_T(T_{soil})_i \times F_v(v) \times D_f)} \right) \times e^{-\tau_{z_i}} \quad (eq.4)$$

where  $S_{C_k}$  is amount of carbon in the soil organic pool (DPM/RPM/BIO for DOC labile pool and HUM for recalcitrant pool) in  $\text{kg C m}^{-2}$  in whole soil,  $K_P$  is DOC production rate in  $\text{day}^{-1}$ ,  $F_S(S)_i$  and  $F_T(T_{soil})_i$  are respectively the rate modifiers due to moisture and temperature, which are controlling decomposition in each soil layer ( $i$ ),  $F_v(v)$  is the fraction of the vegetation. All units are given in Table 2. The moisture and temperature rate modifiers are based on the RothC formulations (Coleman & Jenkinson 2014).  $\tau_z$  is the empirical factor for decrease of C decomposition rates with soil depth, as recently introduced in JULES (Burke et al. 2016).

The DOC production rate is further modified by  $D_f$ , which considers the decrease of SOC decomposition rate as increase of silt plus clay content given in fraction (Parton et al. 1987):

$$D_f = 1 - (0.75 \times (clay + silt)) \quad (eq.5)$$

After decomposition, carbon pools ( $S_C$ ) are updated by the changes in each time step (daily) as follow:

$$\frac{\Delta S_{CDPM}}{\Delta t} = f_{DPM} A_c - R_{DPM} - \sum_{i=1}^{i=4} F_{PDPM_i} \quad (eq.6)$$

$$\frac{\Delta S_{CRPM}}{\Delta t} = (1 - f_{DPM}) A_c - R_{RPM} - \sum_{i=1}^{i=4} F_{PRPM_i} \quad (eq.7)$$

$$\frac{\Delta S_{CBIO}}{\Delta t} = 0.46 (1 - B_R) R_S - R_{BIO} - \sum_{i=1}^{i=4} F_{PBIO_i} + \sum_{i=1}^{i=4} F_{BIOIN_i} \quad (eq.8)$$



$$\frac{\Delta S_{CHUM}}{\Delta t} = 0.54 (1 - B_R) R_S - R_{HUM} - \sum_{i=1}^{i=4} F_{P_{HUM_i}} \quad (eq.9)$$

where in RothC model fraction ( $f_{DPM}$ ) of litter fall ( $A_c$ ) is directed to DPM and RPM depending on vegetation type. C pools are subjected to decomposition. Part of decomposed C as a fraction ( $1-B_R$ ) of total respiration ( $R_s = R_{DPM} + R_{RPM} + R_{BIO} + R_{HUM} + R_{DOC}$ ) is partially feeding microorganisms in soil (BIO) and partially stored as recalcitrant C in soil (HUM) depending on soil texture and the rest ( $B_R$ ) is released to the atmosphere. These parameters were already present in JULES (Clark et al. 2011). In JULES-DOCM the update of carbon pools after DOC production was added (last term of each equation,  $F_{P...}$ , defined in equation 4 above) as well as  $F_{BIO_{IN}}$  the input flux from DOC to BIO pool, described below.

We assume that the decomposition of DOC pools ( $F_D$ ) ( $\text{kg C m}^{-2} \text{ day}^{-1}$ ) also follows first-order kinetics depending on temperature and labile and recalcitrant DOC pool size as follow (arrows e-f Fig. 1):

$$F_{D_{k,i}} = S_{DOC_{k,i}} \times (1 - e^{(-K_{DOC_k} \times F_T(T_{soil})_i)}) \quad (eq.10)$$

where  $S_{DOC_i}$  is the DOC pool size ( $k$  for labile or recalcitrant) in  $\text{kg C m}^{-2}$  and  $K_{DOC_k}$  is the basal decomposition rate of the dissolved DOC ( $k$  for labile or recalcitrant pool) (in  $\text{day}^{-1}$ ) and  $F_T(T_{soil})_i$  is the soil temperature rate modifier within each soil layer (i) same as in eq.4.

Part of decomposed DOC is respired ( $R_{DOC}$  in  $\text{kg C m}^{-2} \text{ day}^{-1}$ , arrow g Fig. 1) and the rest returns to the BIO carbon pool ( $F_{BIO_{IN}}$  in  $\text{kg C m}^{-2} \text{ day}^{-1}$ , arrow h Fig. 1) from each soil layer (i) and DOC pools (k). This proportion is controlled by a CUE parameter (Kalbitz et al. 2003) which is set to 0.5 as a default as in Manzoni et al. (2012).

Hence distribution of decomposed DOC to the BIO pool and respiration will be:

$$F_{BIO_{IN_i}} = (1 - CUE) \times \sum F_{D_{k,i}} \quad (eq.11)$$

$$R_{DOC_{k,i}} = CUE \times \sum F_{D_{k,i}} \quad (eq.12)$$

For adsorption/desorption, a constant sorption equilibrium distribution coefficient ( $K_D$ ) is used to partition DOC in dissolved and adsorbed phases. The assumption is that DOC in the labile or recalcitrant pool is proportionally distributed between adsorbed DOC ( $S_{DOC_{ad}}$ ) and dissolved DOC pools ( $S_{DOC}$  in soluble phase) depending on  $K_D$  from each soil layer(i) and DOC pool (k). Hence if the potentially adsorbed DOC fraction ( $AD_{pot_i}$ ) compared to the size of the actually adsorbed DOC ( $S_{DOC_{ad_{k,i}}}$ ) is positive then this fraction will be adsorbed and added to the adsorbed DOC pool, and if it is negative then this fraction will be desorbed and added to dissolved DOC pool per model time step.

These terms for DOC labile and recalcitrant pools in JULES-DOCM are as follow (arrow: i and j, Fig. 1):

$$AD_{pot_i} = S_{DOC_{k,i}} \times K_D \times \frac{BK}{\theta_{v_i}} \quad (eq.13)$$

$$S_{DOC_{k,i}} = S_{DOC_{k,i}} - (AD_{pot_i} - S_{DOC_{ad_{k,i}}}) \quad (eq.14)$$

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$$S_{DOC_{ad_{k,i}}} = S_{DOC_{ad_{k,i}}} + (AD_{pot_i} - S_{DOC_{ad_{k,i}}}) \quad (eq.15)$$

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where  $S_{DOC_{k,i}}$  is dissolved labile and recalcitrant DOC pools in  $\text{kg C m}^{-2}$ ,  $K_D$  is the distribution factor ( $\text{m}^3 \text{ water kg}^{-1} \text{ soil}$ ),  $BK$  is bulk density ( $\text{kg soil m}^{-3}$ ) and  $\theta_{v_i}$  is the volumetric soil moisture ( $\text{m}^3 \text{ m}^{-3}$ ) and it is considered to be same for DOC labile and recalcitrant pools.

DOC diffusion ( $F_{Diff_{i,j}}$ ) in  $\text{kg C m}^{-2} \text{ day}^{-1}$  between the layers is based on Fick's second law and it is the function of the diffusion coefficient ( $D$ ) in  $\text{m}^2 \text{ day}^{-1}$ , concentration of labile or recalcitrant DOC at different soil depths ( $C_{DOC_{k,i,j}}$ ) in  $\text{kg C m}^{-2}$  and the distance ( $z_{i,j}$ ) between midpoints of soil layers (i: downward flow; j: upward flow) in m (arrow k, Fig. 1):

$$15 \quad F_{Diff_{i,j}} = D \times \frac{\partial^2 C_{DOC_{k,i,j}}}{\partial z_{i,j}^2} \quad (eq.16)$$

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Leaching of the DOC is considered to occur from all 4 DOC soil layers. The top DOC is defined as the first two layers representing the first 35 cm of the soil. The lower two DOC layers represent the sub-soil from 35 cm down to 3 m. Soil leaching at the top DOC layer is dependent on the surface runoff whereas subsurface leaching is dependent on the subsurface runoff. However subsurface runoff is also representing the drainage from the bottom of the 3m soil column, and thus mimics the groundwater base flow, in terms of water as well as in terms of DOC exports. More information on the hydrology of model is given in Gedney & Cox (2003); Clark & Gedney 2008). Both DOC layers leaching fluxes are based on the concentration of dissolved DOC in the soil water. Hence leaching of DOC ( $L$ ) from the dissolved labile and recalcitrant pool within the top (sum of first and second soil layer) - and sub-soil (sum of third and fourth soil layer) (T and S) in  $\text{kg C m}^{-2} \text{ day}^{-1}$  is calculated as follows (arrow l, Fig.1):

$$25 \quad L_T = S_{DOC_{k,h}} \times \frac{Roff_{surf}}{T_{s_i}} \quad (eq.17)$$

$$L_S = S_{DOC_{k,h}} \times \frac{Roff_{sub}}{T_{s_i}} \quad (eq.18)$$

where  $S_{DOC_{k,h}}$  is the DOC quantity in the dissolved labile and recalcitrant pool ( $h$  for top or sub soil),  $Roff_{surf}$  is the surface runoff,  $Roff_{sub}$  is the subsurface runoff (both  $\text{kg m}^{-2} \text{ day}^{-1}$ ) and  $T_{Si}$  (defined in code as  $\theta_s$ ) is the soil moisture in each soil layer ( $i$ ) ( $\text{kg m}^{-2}$ ).

Hence dissolved and adsorbed DOC pools are updated as follow:

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$$\frac{\Delta S_{DOC_k}}{\Delta t} = F_{P_{k,i}} + AD_{pot_i} + F_{Diff_i} - F_{D_{k,i}} - L_T - L_S \quad (eq.19)$$

Values of the default DOC model parameters are given in Table 1.

## 10 2.3 Sites description

Two data levels were provided in order to test the model performance. Level 1, including Hainich, Carlow and Brasschaat which included the carbon fluxes and continuous DOC measurements from soil water from 3 to 10 years period, and level 2, including Turkey Point 89 (TP89) and Guandaushi with fewer C fluxes measurements and discontinuous DOC measurements (Table 3). Location of sites are given in Figure 2.

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### 2.3.1 Hainich

The site “Hainich”, located in Germany – National park Hainich, (51°04' 45"N, 10°27'07"E), is covered by an old-growth deciduous forest dominated by *Fagus sylvatica* and intermixed with *Fraxinus excelsior* and *Acer pseudoplatanus* (Mund et al. 2010). The soil class at this site is Eutric Cambisol with a high clay content and high biological activity, as illustrated by a mull or F-Mull organic layer (Table 4). The mean annual air temperature is 7.5-8°C and the annual precipitation is in the range of 750-800 mm  $\text{yr}^{-1}$  (Kutsch et al. 2010). At this site, soil solution samples were taken at three depths (5, 10 and 20 cm) using ceramic suction plates positioned at four different plots within the site. Samples were obtained by applying a tension of 100 hPa after each bi-weekly sampling occasion.

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### 2.3.2 Carlow

The site “Carlow” is located in Ireland – County Carlow, (52° 52'N, 6° 54'W). The land cover is grassland, the soil class is Calcic Luvisol. This sandy loamy soil has a uniform profile and is well-drained (Table 4). The climate is characterized by a mean annual air temperature of 9.3°C and a mean annual precipitation of 823 mm  $\text{yr}^{-1}$  (Walmsley et al. 2011). DOC samples were collected from at two locations separated 150 m from each other, using 20 suction cups per location, with ten of these

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cups installed directly beneath the rooting zone and the other ten at a depth of 0.7 m. Samples were obtained by applying a tension of 400 hPa after each bi-weekly sampling occasion (Walmsley 2009).

### 2.3.3 Brasschaat

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The site “Brasschaat” is located in Belgium and covered by mixed coniferous/deciduous (De Inslag) forest, (51°18’33" N, 4°31’14" E) with stands of old Scots Pine (*Pinus sylvestris*) (Janssens et al. 1999). The temperate maritime climate is characterized by a mean annual air temperature of 11.1°C and a mean annual precipitation of 824 mm yr<sup>-1</sup> (Gielen et al. 2010). The soil class was defined as Albic Hypoluvic Arenosol (Table 4). The profile usually exhibits a high soil moisture, but due to the sandy texture and rapid hydraulic conductivity in upper horizons, it is rarely saturated (Gielen et al. 2011).

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DOC samples were collected at three horizons of Al/Ap, A/E and Cg (Soil Classification Working Group 1998) referred to 10,35 and 75cm depth, by means of ceramic suction cups on a biweekly interval. Two days prior to sample collection a tension of 600 hPa was applied to each suction cup. Samples were collected at three locations and pooled into one composite sample per layer for analysis (Gielen et al. 2011).

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### 2.3.4 Turkey Point 89

The site “Turkey Point 89 (TP89)”, located in southern Ontario – Canada, (42°77’57"N, 80°45’09"E), is covered by an evergreen needleleaf forest dominated by Eastern White pine (*Pinus strobus* L.) mixed with few stands of Oak, Paper birch, Wild black cherry and Red pine (Peichl & Arain 2006) established in 1989 on agricultural lands (Peichl, Brodeur, et al. 2010). The mean annual air temperature is 8.1°C and mean annual precipitation is 832 mm yr<sup>-1</sup> (Peichl & Arain 2006). The soil class at this site is Gleyed Brunisolic Luvisol and due to the high sand content, it is well drained and has a low to moderated water holding capacity (Peichl, Brodeur, et al. 2010; Presant, E.W., Acton 1984). DOC sampling was attempted in monthly intervals at three depths of 25, 50 and 100 cm by means of porous suction cups, however, due to the dry sandy soils, samples could only be retrieved for 5 separate days of sampling after heavy rain fall events on 29-Nov-2004, 3-May-2005, 16-Jun-2005, 29-Jun-2005, 14-Oct-2005 (Peichl et al. 2007).

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### 2.3.5 Guandaushi

The site “Guandaushi” is located in central Taiwan, (23° 8'N, 120° 8'E). The climate is characterized by distinct rainy and dry seasons and a mean annual air temperature of 22.4°C and annual precipitation in the range of 2300 to 2700 mm yr<sup>-1</sup>. The land cover is subtropical mixed hardwood forest including three stands of natural hardwood and secondary hardwood on light loam textured soil and Chinese fir (*Cunninghamia lanceolate*) on heavy clay textured soil. DOC samples were collected at three depths of 15, 30 and 60 cm in three locations at bi-weekly interval by means of ceramic suction cups.

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## 2.4 Model input and setting

Model performance was tested against observed data from Guanduashi and four FLUXNET sites (Hainich, Carlow, Brasschaat and Turkey Point-89). The FLUXNET database provides on-site meteorological data for each site that could be used as forcing for simulations in JULES. However, we had to use the global WATCH dataset (Weedon et al. 2010) as forcing for Guandaushi site where no on-site data was available. However, both forcing data were checked for any missing data and it was gap filled by linear interpolation. The meteorological forcing is provided at the measurement site level (no explicit spatial resolution) and includes the downward shortwave and longwave radiation at the surface ( $W\ m^{-2}$ ), rainfall ( $kg\ m^{-2}\ s^{-1}$ ), snowfall ( $kg\ m^{-2}\ s^{-1}$ ), wind speed ( $m\ s^{-1}$ ), atmospheric temperature (K), atmospheric specific humidity ( $kg\ kg^{-1}$ ) and air pressure at the surface (Pa) at half an hour time step (Best et al. 2011).

For Brasschaat, additional model parameters such as BK and clay were taken from Janssens et al. (1999). The model was first spun-up looping over period 1996 to 2014 until all the soil variables reached a steady state. For Hainich, site parameters were taken from Kutsch et al. (2010). The spin-up was run looping 300 times over the years 2004 to 2014. For Carlow, site parameters were taken from Walmsley (2009) and Kindler & Siemens (2010). The spin-up was run looping 300 times over the years 2004-2009. For Turkey Point-89, site parameters were taken from Peichl & Arain (2006) and spin-up was run looping 300 times over the years 2002-2007. For Guandaushi, site vegetation parameters were taken from Liu & Sheu (2003) and soil parameters from HWSD global data (Nachtergaele et al. 2010) and spin-up was run looping 300 times over years 1990 to 2000. The evaluation of model was performed on plot-scale, using climate forcing data, soil and land cover consistent with the site, no horizontal spatial dimension was involved.

## 2.5 Sensitivity test

In order to test the sensitivity of DOC related model parameters on the DOC concentration in different depths of the soil profile, simulations were performed with varying values for  $z_0$ ,  $\tau_z$  and DOC controlling parameters such as  $K_{DOC\ (labile)}$ ,  $K_{DOC\ (recalcitrant)}$ , slope parameter of  $D_f$ ,  $CUE$ ,  $K_D$  and  $D$  (Table 1).

In total, 16 runs were performed by modifying each parameter once by increasing it 50% and once by decreasing it by 50%, except for the slope parameter controlling  $D_f$  (eq. 5) which was changed by 33% to remain within the physical boundaries. In order to do the comparison with measurements, runs were performed for 3 meters soil depth for the periods that measurements were available. Hence, Brasschaat runs were performed for the years 2006-2010, Hainich runs for the years 2005-2014 and Carlow runs for the years 2006-2008.

## 2.6 Statistical analysis

In order to test the model performance, with regard to simulated C stock and fluxes, we used an ANOVA (Analysis of variance) test to compare the model results from the default set of parameters against measurements. In order to test the

parameter impact on the simulated DOC concentrations, we computed the RMSE values from each set of model parameter configurations.

### 3 Results

#### 3.1 Validation of carbon concentration and fluxes

To examine the performance of soil DOC simulations, it is first necessary to explore other carbon fluxes which link to soil DOC pools. The first flux to be validated is the gross primary production (GPP), for which we have observed values (Table 3). The modelled mean GPP for Brasschaat and Carlow was significantly lower than measurements with  $867 \pm 25 \text{ g C m}^{-2} \text{ year}^{-1}$  compared to  $1173.3 \pm 91 \text{ g C m}^{-2} \text{ year}^{-1}$  and  $903.2 \text{ g C m}^{-2} \text{ year}^{-1}$  compared to  $1165.3 \text{ g C m}^{-2} \text{ year}^{-1}$  ( $p < 0.05$ , Table S3), respectively. For Turkey Point 89 and Hainich, the measured GPP was in line with our model results with  $1731.5 \pm 108 \text{ g C m}^{-2} \text{ year}^{-1}$  and  $1606.74 \pm 101 \text{ g C m}^{-2} \text{ year}^{-1}$  compared to  $1635.1 \pm 62 \text{ g C m}^{-2} \text{ year}^{-1}$  and  $1455 \pm 167 \text{ g C m}^{-2} \text{ year}^{-1}$  ( $p = 0.162$ , Table S3). The modelled NPP was higher than observed values for Hainich and for Turkey Point-89, while it was lower than observed values for Brasschaat (Table 5).

Total soil respiration measurements were available for Brasschaat, Hainich and Turkey Point-89 (Table 3) and were compared with the modelled outputs. The simulated values were close to observed values at Hainich, while the modelled values for Brasschaat were significantly higher ( $p\text{-value} < 0.05$ , Table S3) and for Turkey Point-89 higher ( $p\text{-value} = 0.0896$ , Table S3), than the observed values (Table 5).

Finally, we compared the SOC in measurements and model outputs, where the measurements from Brasschaat for 100 cm, Hainich for 60 cm, Carlow for 50 cm and Turkey Point-89 for 15cm (A-horizon) of soil were available. The modelled SOC stock for Brasschaat in the first 100 cm and for Hainich down to 60 cm were slightly lower than the observations, while for Carlow the simulated stocks down to 50 cm and for Turkey Point-89 the simulated stocks down to 15 cm were higher than the observed stocks (Table 5).

#### 3.2 DOC simulations

In general, JULES-DOCM was capable of reproducing the DOC concentrations at all the tested sites using the default set of parameters (Table 1) chosen as representative for the top soil (Fig. 3 Level 1 sites, Fig. 4 level 2 sites). For Hainich, the simulated average values and value range were close to observed values at 10 cm and 20 cm (Table 5, RMSE values for 10 cm and 20 cm are  $3.0$  and  $2.5 \text{ mg L}^{-1}$  respectively). For Brasschaat, the simulation underestimated DOC concentrations at all depths, but with an increasing underestimation with soil depth (Table 5, RMSE values for 10, 35 and 75 cm are  $22.9$ ,  $18.4$  and  $16.8 \text{ mg L}^{-1}$  respectively). For Carlow, the modelled and measured values were close at depths of 10 cm and 77 cm, but

strongly underestimated at the intermediate depth of 28 cm (Table 5, RMSE values for 10, 10-38 and 28-77 cm are 3, 10.2 and 1.5 mg L<sup>-1</sup> respectively). At Turkey Point-89, the modelled and observed values were close at 25cm depth, but the DOC concentration average over the profile down to 100 cm was overestimated (Table 5). For Guandaushi, DOC measurements from three different stands (Natural hardwood, secondary hardwood and Chinese fir) values were compared with modelled values. The model values for a depth of 15 cm were closer to observed values for Chinese fir than for natural hardwood or secondary hardwood sites. For 30cm depth, the simulated DOC concentration was substantially lower than the measured DOC averaging over three stands in Guandaushi (Table 5).

Overall, the model was capable of reproducing the seasonality of DOC concentrations for the European sites where long-term observation data are available (Fig. 5). However, at Braschaat the simulated DOC peaked from April-July while observed DOC peaked from July-September.

We also examined the hydrology of the model and its interaction with DOC concentration and leaching (e.g. Hainich - Fig. 6; other sites are plotted in Fig. S3). It can be seen for the period 2005 to 2014 that during heavy precipitation, high runoff was produced which caused the higher leaching, and the consequence was a drop in the DOC concentration in 3 meters of soil.

### 3.3 Sensitivity tests

Sensitivity to model parameters was tested on the three European sites where a representative time-series of observed DOC concentrations was available (e.g. Hainich-10cm, Fig. 7). The results indicate that among all the parameters in all three sites, the model shows the highest sensitivity to SOC vertical profile, controlled by parameter  $z_0$  (eq. 1), and the changing of SOC decomposition rate with soil depth, parameter,  $\tau_z$  (eq. 4) (p-values < 0.05, Table S6). Among the DOC controlling parameters, the model shows the highest sensitivity to the basal decomposition rate of recalcitrant DOC ( $K_{DOC (recalcitrant)}$ ) (eq.10), which is the inverse of the residence time of DOC in the recalcitrant pool.

The sensitivity of the model to each of these parameters was different at each site. For Hainich, the highest sensitivity was assigned to  $\tau_z$ . Here, a change in  $\tau_z$  by 50% leads to a 36% change in the mean DOC within 3 m, while a 50% change in  $K_{DOC (recalcitrant)}$  leads to a 29% change and global  $z_0$  leads to a 25% change in simulated DOC concentrations (Fig 8a). The closest value for the mean DOC in 10 cm in Hainich (8.8 mg L<sup>-1</sup>) to the measurement was produced by the default set (8.9 mg L<sup>-1</sup>), while the highest value for DOC was reached with the 50% increase in  $\tau_z$  (12.7 mg L<sup>-1</sup>) and the lowest DOC value was produced with 50% decrease in  $\tau_z$  (4.7 mg L<sup>-1</sup>). In contrast to that, at a depth of 20 cm, the closest value to the mean of measured DOC (5.6 mg L<sup>-1</sup>) was produced by 50% decrease in  $K_{DOC (recalcitrant)}$  (4.9 mg L<sup>-1</sup>) (Fig. 9-a).

In Brasschaat, the highest sensitivity was to  $z_0$ , closely followed by  $\tau_z$  and  $K_{DOC (recalcitrant)}$ . A 50% change in each of these parameters led to a 36-40% change in DOC concentration over the 3 meters of soil profile (Fig. 8-b). At 10 cm, the closest value to measurements mean (39.4 mg L<sup>-1</sup>) was produced by 50% increase in  $\tau_z$  (39.2 mg L<sup>-1</sup>). At 35 cm depth, the closest

value to mean measurement ( $29.3 \text{ mg L}^{-1}$ ) was calculated by 50% increase in  $K_{DOC}(\text{recalcitrant})$  ( $16.2 \text{ mg L}^{-1}$ ) which was also the highest simulated value as well. At 75 cm, the closest value to mean of DOC measurement ( $22.0 \text{ mg L}^{-1}$ ) was produced by 50% increase in  $K_{DOC}(\text{recalcitrant})$  ( $8.1 \text{ mg L}^{-1}$ ) as it was the highest of the simulated values (Fig. 9-b).

For Carlow, the most sensitive parameters were  $\tau_z$  and  $K_{DOC}(\text{recalcitrant})$ : a 50% change in those parameters leads to a 31.5% and 27.4% in simulate DOC. In contrast to the other sites, global  $z_0$  leads to a low but still significant positive change of 6.5% in simulated DOC within 3 meters of soil (p-value  $<0.05$ , Table S6) (Fig. 8-c). In 10cm, the closest modelled value to the mean measurement ( $5.7 \text{ mg L}^{-1}$ ) was produced by default parameter set ( $5.8 \text{ mg L}^{-1}$ ). Between 10 to 28 cm all the parameter sets underrepresented the DOC concentration mean measurement ( $13.1 \text{ mg L}^{-1}$ ) and the closest and highest value was produced by 50% in  $\tau_z$  ( $3.8 \text{ mg L}^{-1}$ ). For 28 to 77cm, the closest value to the measurement ( $4.8 \text{ mg L}^{-1}$ ) was calculated by increasing  $\tau_z$  by 50% ( $4.5 \text{ mg L}^{-1}$ ) (Fig. 9-c).

## 4 Discussion

### 4.1 Measurements versus model simulations

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Overall, JULES-DOCM reproduced the range of GPP for most of our sites to an acceptable degree. At some sites, due to over/underestimated autotrophic respiration, the NPP and total respiration values were slightly different than measurements. Consequently, the modelled carbon stocks were different from the measurements in most of the sites, but yet capable of representing the general patterns that were observed in the measurements.

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In Brasschaat, the modelled SOC was lower than the measurements, which could be due to the underestimated NPP (Table 5) and, as a consequence, the underestimated litter input, but also due to the overestimated soil respiration and SOC decomposition rates. The underestimation of SOC as a source of DOC led to a general underestimation of DOC. Nevertheless, the decrease of relative DOC concentration through soil is consistent with the observations.

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In Hainich, a slightly overestimated NPP partly counter-balanced the overestimated soil respiration. Nevertheless, the SOC concentration simulated down to 60 cm was lower than the measurement at this depth. As we did not have observations of SOC down to 3 meters, we cannot certainly say if the simulated total SOC stock ( $13.7 \text{ kg C m}^{-2}$ ) over the whole soil column is close to the reality or not. Some of the controlling parameters like DOC basal decomposition rates are kept constant over the soil profile in our simulation, while they are maybe not constant with depth in the real world, perhaps due to priming effects (Guenet et al. 2010). That could explain why at Hainich, the simulated and observed DOC concentrations are very close at 10 cm depth, while they differ more at 20 cm depth.

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In Carlow, the slight overestimation of GPP led to the overestimated SOC concentrations down to 50 cm, whilst again we cannot say with certainty that the whole SOC stock is overestimated, as the SOC stock has not been measured down to three meters. Some sources suggest that the SOC in Carlow grassland could be higher than the reported value in our reference, if we calculate the C in soil based on the fraction of loss of ignition (LOI) (Walmsley 2009; Hoogsteen et al. 2015). As Carlow



is our only grassland biome site, additional data from different study sites would be valuable to achieve a more representative parametrization of soil carbon processes under grassland. One of the parameters to be optimized for such sites could be CUE which has a strong impact on the stocks and fluxes. Also, since the measured values for NPP or soil respiration for this site were not available to us, we were unable to assess whether we over- or underestimated these fluxes and if this could have potentially biased our SOC stock simulations. DOC measurements were provided from two plots which were placed on different terrain positions. The measurements from plot 2 (150 meter in south-westerly direction from plot 1) at 10 to 28 cm depth had a higher DOC concentration than plot 1 at the 10 cm (Walmsley 2009). This could be the result of small scale variations related to terrain position, which can be related to different soil moisture regimes and lateral import of DOC. It is not possible to represent such small-scale variation in global models like JULES-DOCM.

At Turkey Point-89, the simulated GPP is close to the observations, while NPP is slightly overestimated. The simulated soil respiration and decomposition rates are higher than observed values. The overestimated SOC concentration in the top soil could be the result of an overestimated depth gradient in SOC concentration, which in our simulations is derived from global data (Jobbágy & Jackson 2000). Also, we simulated the steady state SOC profile for forest vegetation, whereas the forest stand at the site is relatively young and succeeded agricultural land use in 1989, and thus, the SOC profile is likely not representative for a forest site. The overestimated DOC concentration for 100 cm depth may be due to this change in land use, which was not taken into account during simulations, providing more C input for DOC production. At this site, the observed higher soil moisture in the deeper profile could indicate a potentially high advection of DOC to the lower layers (Peichl, Arain, et al. 2010). This could be another reason for the lower DOC in 100 cm from measured compared to the modelled results.

In Gundaushi due to the lack of SOC, or vegetation carbon fluxes measurements from the site, we have no information on SOC concentrations and stocks. The lower values of DOC from our model compared to the measurements could be due to: Firstly, the high temporal variability of observed concentrations (large standard deviation for all the depths from the three stands). Second, the high value of DOC input from rainfall, which is not represented in JULES-DOCM (Liu & Sheu 2003). Recent studies have indicated that including this flux in models can have a significant impact on the DOC in soil (Lauerwald et al. 2017).

As there are no measurements of lateral leaching of DOC from soil to the river, our evaluation of this flux is based on the simulated DOC concentration and runoff. Hence as the simulated hydrology of the JULES model has been evaluated previously (Gedney, N. , Cox 2003; Clark & Gedney 2008), in this study, we assume that we will get robust estimates of DOC leaching by multiplying simulated concentration by runoff, as long as simulated DOC concentrations can be validated.

Overall, besides over/underestimation of DOC at some sites, the model was capable of representing the trend of DOC concentration at different depths when comparing to the measurements at all the sites.

## 4.2 Sensitivity analysis

The sensitivity tests indicate that the parameters controlling SOC concentrations in the soil profile ( $Z_0$  and  $\tau_z$ ) and the recalcitrant DOC residence time ( $K_{DOC(\text{recalcitrant})}$ ) have the most significant effect on soil DOC concentration, which indicates the importance of factors controlling DOC sources. Nevertheless, DOC related model parameters such as basal DOC decomposition rate are constant over different depths, which could be the reason for the difference between the modelled and measured values, especially in the deeper soil layers. Hence, it is important to introduce a depth-dependence decay rate for these parameters.

One limitation in our simulation is that we use a single, calibrated value for recalcitrant DOC residence time, which is the most sensitive DOC controlling parameter. It has been shown that this parameter can vary with biodegradability of SOC and litter under different PFTs and at different sites (Kalbitz et al. 2003; Turgeon 2008). However, more detailed data for different biomes is needed for calibrating different residence times for different PFTs. *We note that our sensitivity analysis, changing one parameter at a time, does not investigate the potential interactions between different parameters.*

## 5 Conclusion

Applying a carbon cycle model that integrates the whole continuum from land to ocean to atmosphere provides a better understanding of the Earth's carbon cycle and makes more reliable future projections. In this study, we presented DOC related processes in JULES, JULES-DOCM, which includes the DOC produced in the soil down to three meters and its subsequent fate including its decomposition and release as  $\text{CO}_2$  to the atmosphere, and its export to the river network via leaching in different ecosystems. Results show that the model is capable of representing the DOC stocks, processes and its export to the riverine systems from different ecosystems. In future, our developments in the representation of DOC leaching will lead to a model approach integrating terrestrial and aquatic C cycling. However, more field data are still required to improve the model parametrization and performance.

### Code availability

The code written for this version of JULES can be found at:

[https://code.metoffice.gov.uk/svn/jules/main/branches/dev/mahdinakhavali/vn4.4\\_JULES\\_DOCM/](https://code.metoffice.gov.uk/svn/jules/main/branches/dev/mahdinakhavali/vn4.4_JULES_DOCM/) (registration required)

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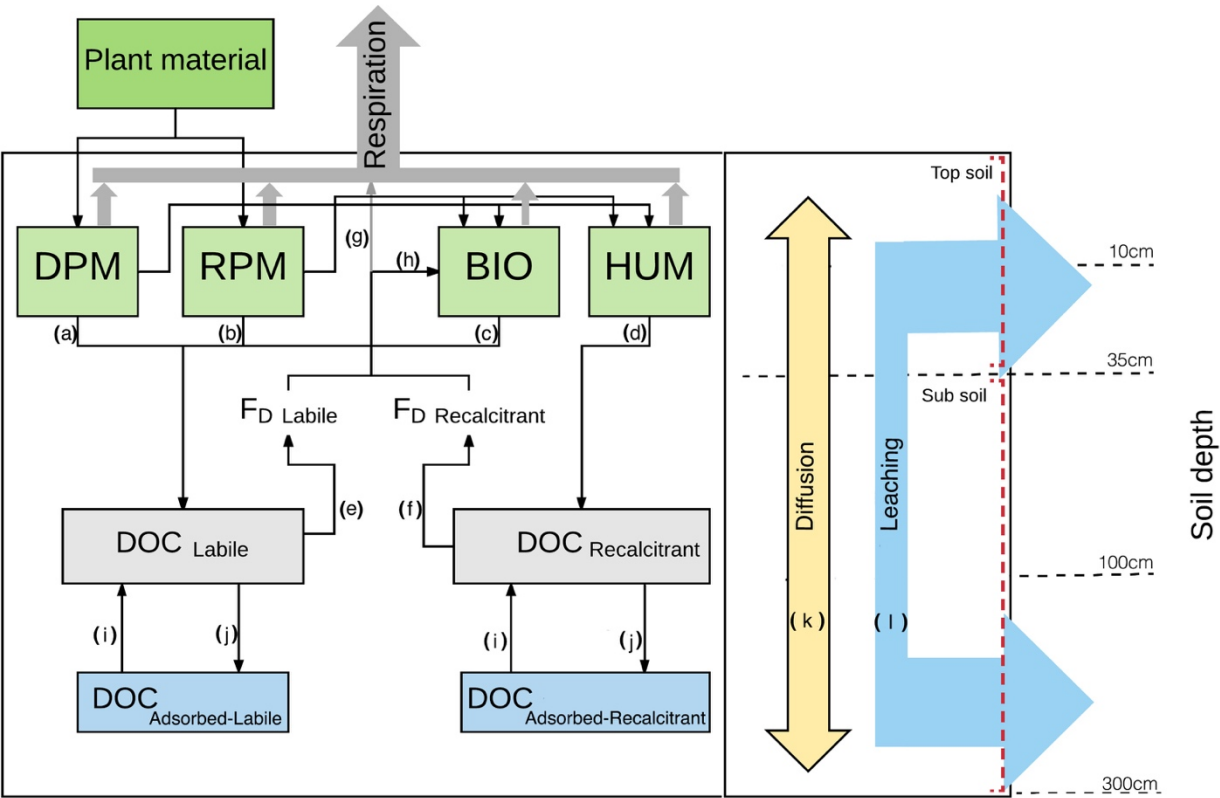


Figure 1. JULES-DOCM model structure

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Figure 2. Study sites

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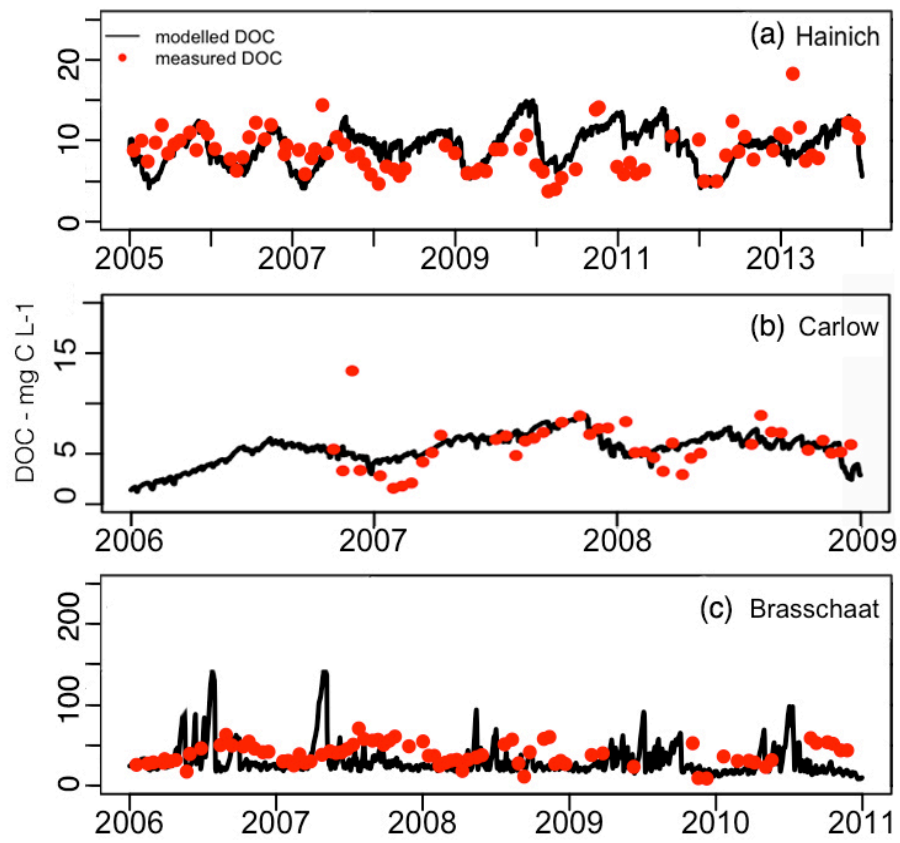


Figure 3. DOC concentration (mg C L<sup>-1</sup>) at 10 cm depth measured (red dots) and simulated (black lines) for (a) Hainich, (b) Carlow, and (c) Brasschaat. Results for other depths are given in Figure S2.

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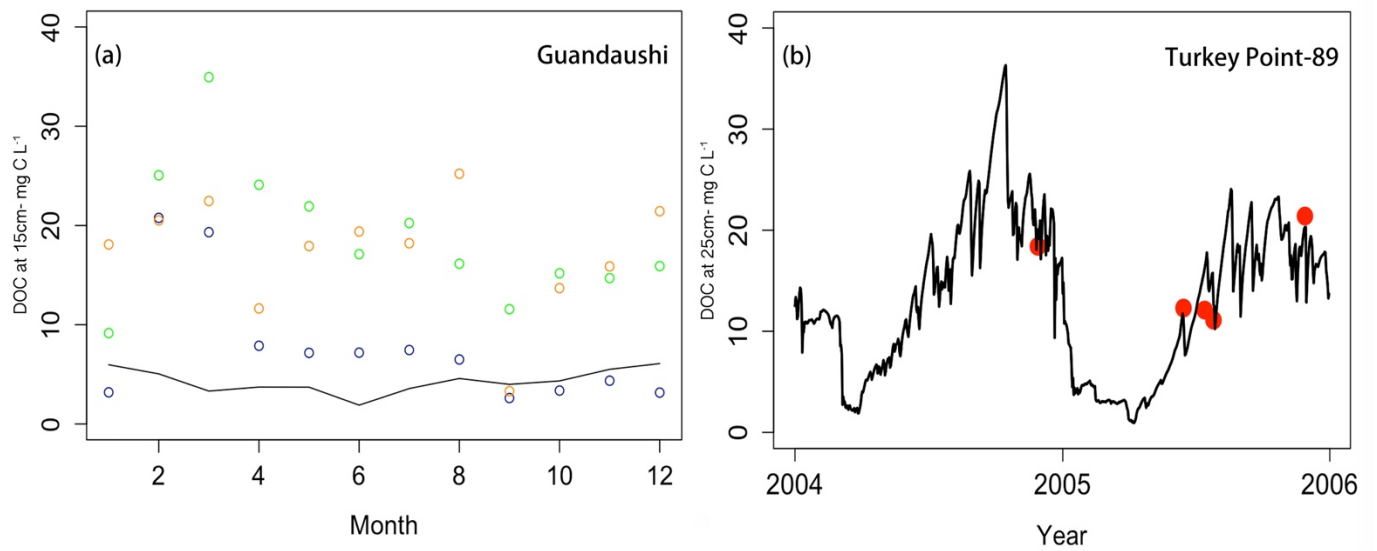


Figure 4. DOC concentration (mg C L<sup>-1</sup>) for (a) Guandaushi at 15 cm measured (black circle: Chinese Fir, green circle: natural hardwood, orange circle: secondary wood) and simulated (black lines) and for (b) Turkey Point 89 at 25 cm measured (red dots) and simulated (black lines). Results for other depths are given in Figure S2.

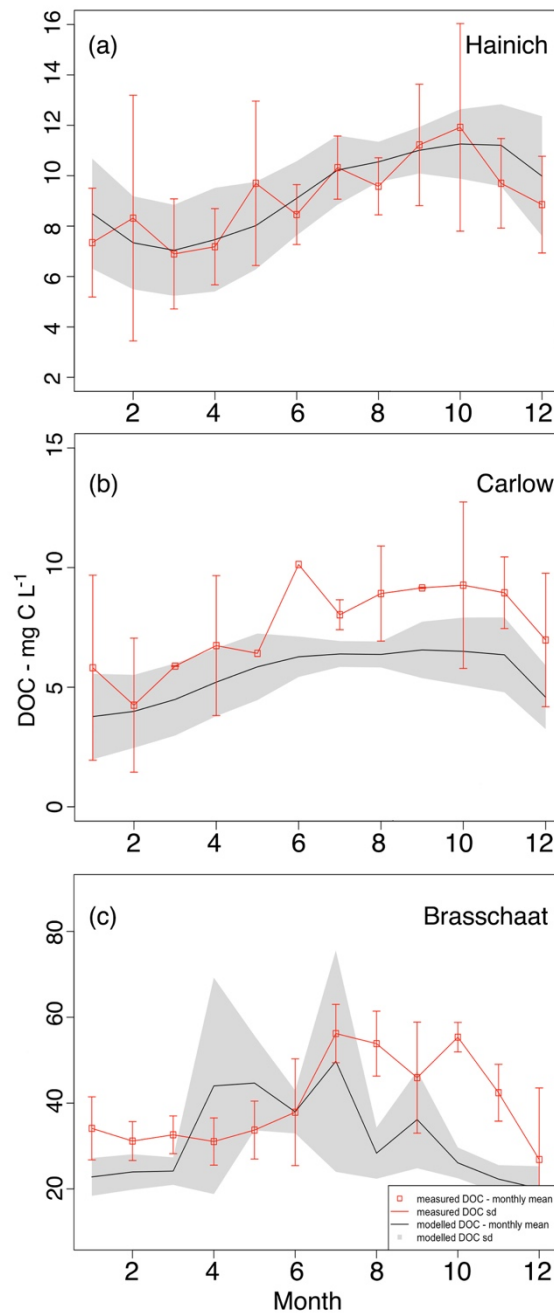
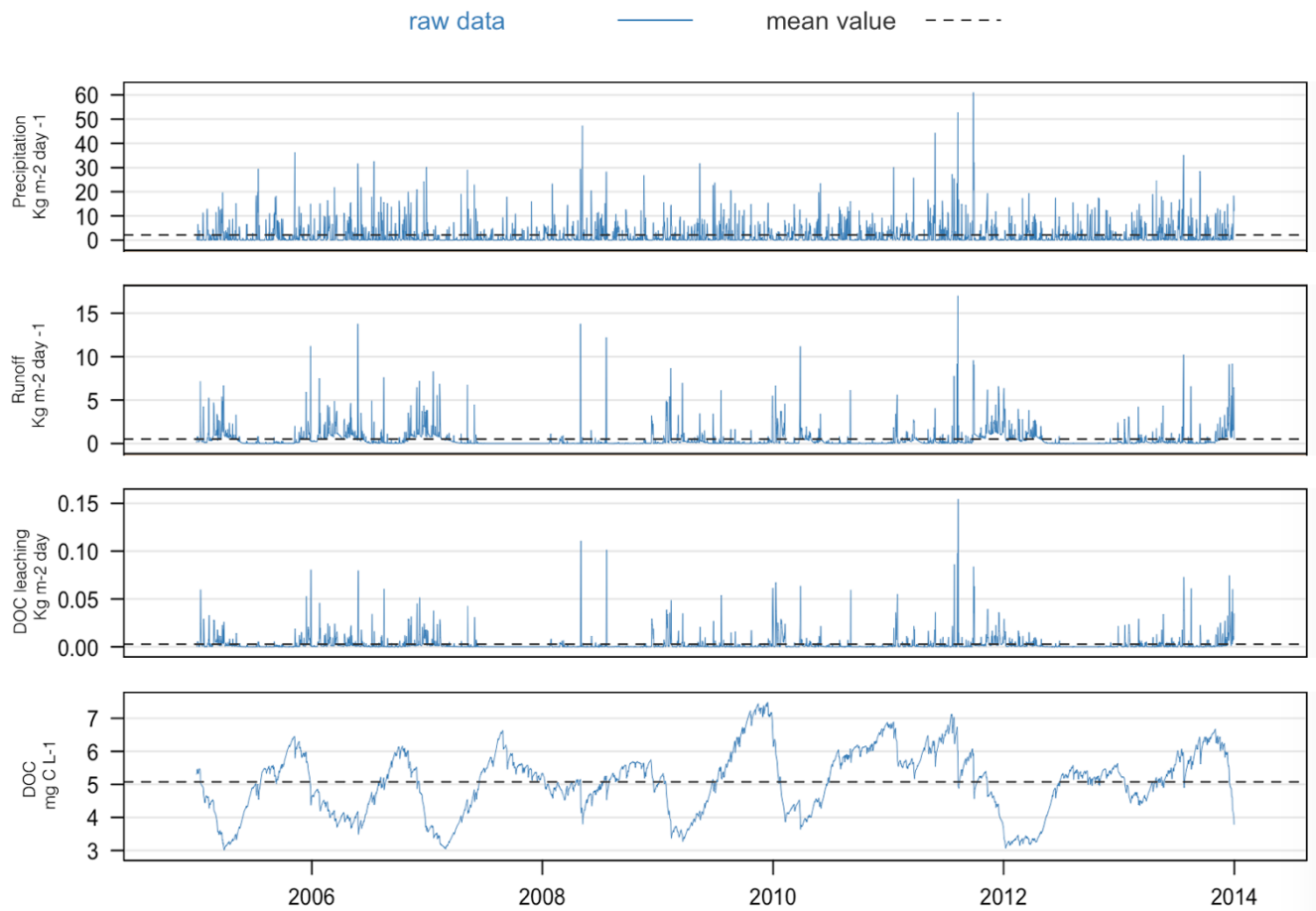


Figure 5. a) Monthly DOC (mg C L<sup>-1</sup>) at 10 cm in Level 1- sites modelled (black line: mean, grey line: standard deviation) versus measured (red square: mean, red line: standard deviation) for studied period (a) Hainich averaging from 2005-2014 (b) Carlow, averaging from 2006-2008 (c) Brasschaat, averaging from 2006 –2010.

5 Results for other depths are given in Figure S6.



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Figure 6. Observed precipitation, simulated runoff, DOC leaching and DOC concentration in Hainich from 2006 to 2013 indicating the relation between the averaged DOC concentrations at 3 m of soil with leaching as a result of runoff that follows large precipitation events.

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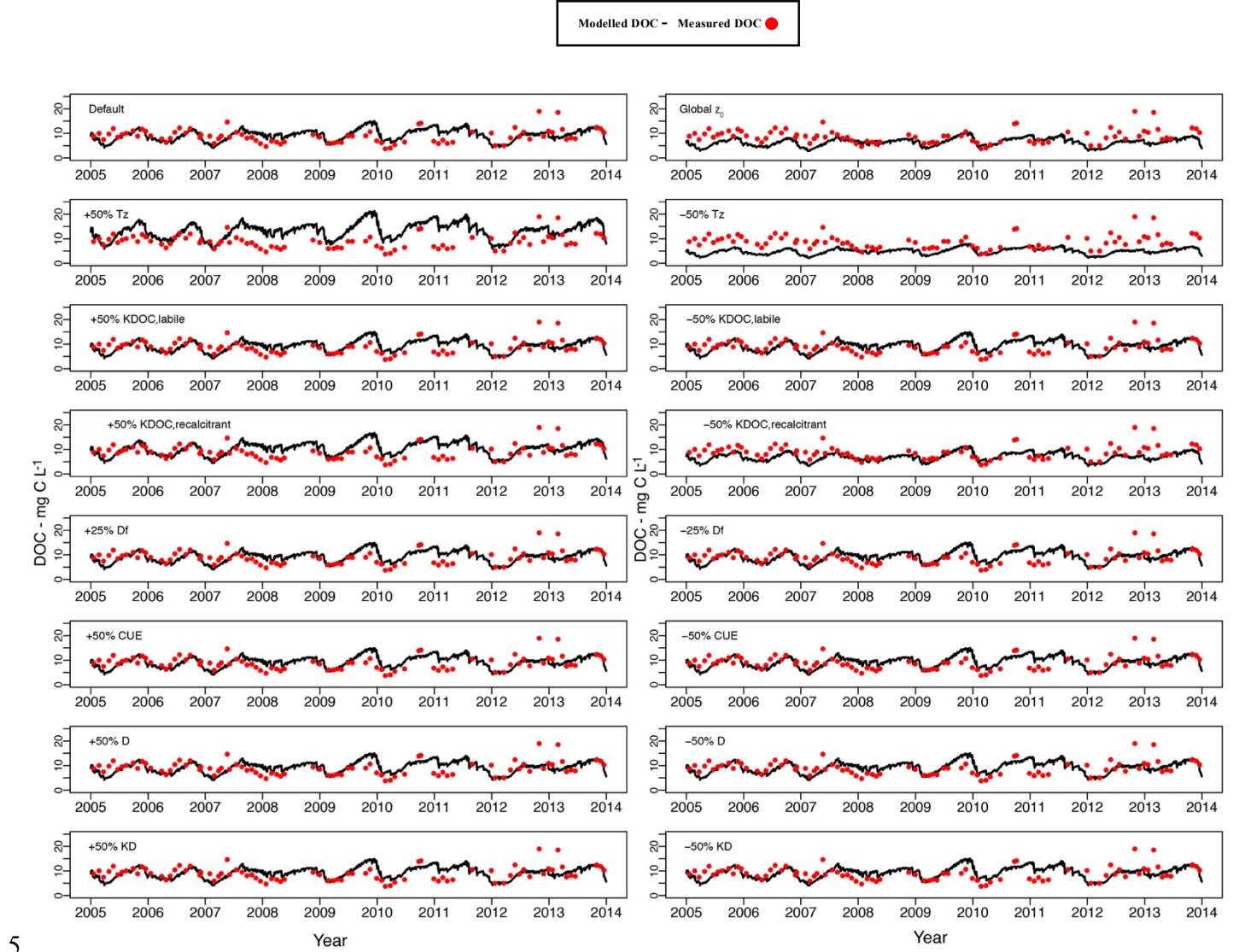


Figure 7. DOC concentration (mg C L<sup>-1</sup>) simulated with sensitivity parameter sets (black line) versus measured (red dot) at 10 cm depth in Hainich for period 2004-2013. Parameter sets description and values are given in Table 1. Results for other sites are given in Figure S1.

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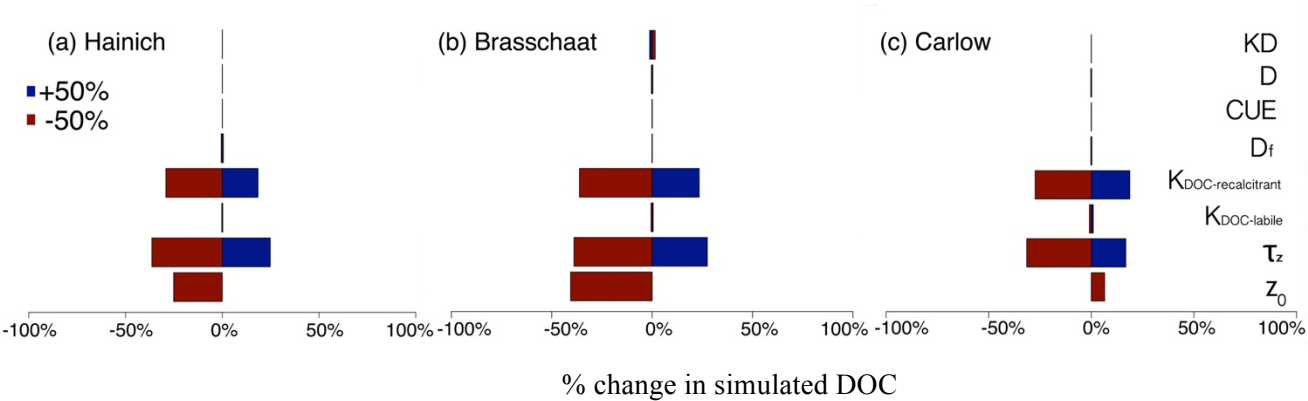


Figure 8. Relative change in simulated DOC (%) for a +50% (blue) and -50% (red) change in each parameter for level 1- sites: (a) Hainich, (b) Brasschaat and (c) Carlow. Values are given in Table S5.

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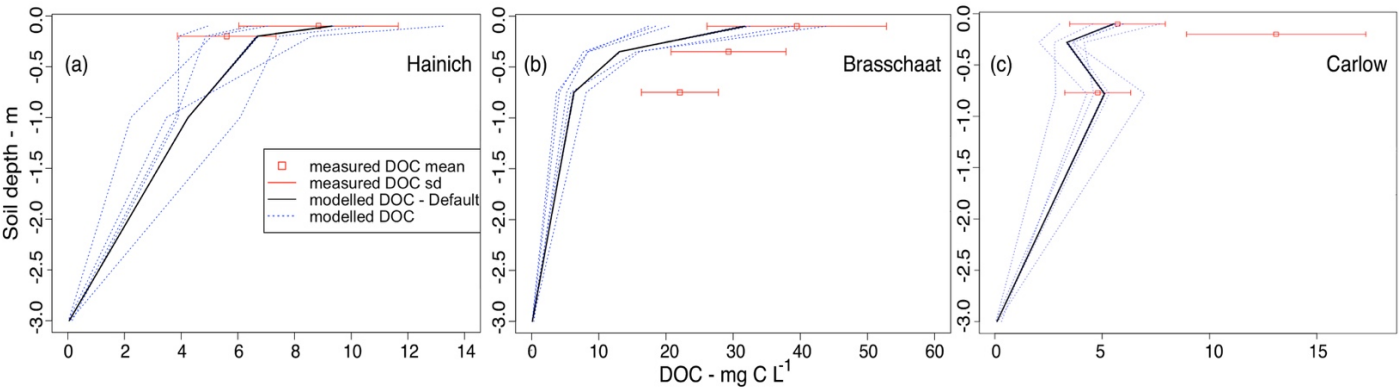


Figure 9. DOC concentration (mg C L<sup>-1</sup>) in 3 m soil depth at level 1-sites modelled (black line: default parameter set; blue dashed line: sensitivity test parameter set) vs. measured (red square: mean; red line: standard deviation) for (a) Hainich (b) Brasschaat (c) Carlow. Plot of each parameter in 3 m soil depth in Figure S5.

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Table 1. DOC relevant parameters in JULES-DOCM model

Parameter	Description	Value	Unit	Sensitivity test values (+/-)	
Carbon parameters					
$z_0$	e-folding depth of carbon content within 1 meter of soil <sup>1</sup>	Values range (65.68 -167.13)	m <sup>-1</sup>	PFT based	109.55
$\tau_z$	Decay of Carbon decomposition with depth (z) <sup>2</sup>	2	m <sup>-1</sup>	3.0	1.0
DOC parameters					
$K_P$	Rate constant for DOC production specific to each carbon pool <sup>3</sup>	1e-4, 5e-6, 5e-5, 2e-6	day <sup>-1</sup>	-	-
$K_{DOC\ (labile)}$	Basal decomposition rate of dissolved DOC labile pool <sup>4</sup>	3.0 Value range (0.46-100)	days	4.5	1.5
$K_{DOC\ (recalcitrant)}$	Basal decomposition rate of dissolved DOC recalcitrant pool <sup>5</sup>	600.0 Value range (66-5000)	days	900.0	300.0
<i>slope parameter of <math>D_f</math></i>	<i>slope parameter controlling DOC production/decomposition modifier depending on clay and silt fraction<sup>6</sup></i>	0.75	-	1.0	0.5
$CUE$	Carbon use efficiency <sup>7</sup>	0.5	-	0.75	0.25
$K_D$	Distribution coefficient of adsorbed DOC <sup>8</sup>	8.05e-6	m <sup>3</sup> water kg <sup>-1</sup> soil	1.207e-4	4.025e-6
$D$	DOC diffusion coefficient <sup>9</sup>	1.062e-05	m <sup>2</sup> day <sup>-1</sup>	1.594e-05	5.313e-06

<sup>1</sup> Jobbágy & Jackson 2000<sup>2</sup> Koven et al. 2013; Burke et al. 2016<sup>3</sup> Jo Smith et al. 2010<sup>4</sup> Kalbitz et al. 2003; Turgeon 2008<sup>5</sup> Kalbitz et al. 2003; Turgeon 2008<sup>6</sup> Parton, W et al. 1987<sup>7</sup> Manzoni et al. 2012<sup>8</sup> Moore et al. 1992<sup>9</sup> Ota et al. 2013



Table 2. Symbols definition and units

Symbol	Units	Definition
$BK$	$\text{kg m}^{-3}$	Bulk density
$B_R$		Fraction of soil respiration which is respired
$\beta_z$	$\text{m}^{-1}$	Carbon distribution with depth, depending on biome
CUE		Carbon use efficiency
$C_{\text{DOC}}$	$\text{kg C m}^{-2}$	Amount of DOC subjected to transport by diffusion
$D$	$\text{m}^2 \text{ day}^{-1}$	DOC diffusion coefficient
$D_f$		DOC production / decomposition modifier depending on clay and silt fraction
$dz$	$\text{m}$	Soil layer thickness
$\Delta S_{\text{BIO}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Biomass carbon pool update
$\Delta S_{\text{DPM}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Decomposable plant material carbon pool update
$\Delta S_{\text{HUM}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Humus carbon pool update
$\Delta S_{\text{RPM}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Resistant plant material carbon pool update
$\Delta S_{\text{DOC}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Labile and recalcitrant DOC pools update
$AD_{\text{pot}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Adsorbed/desorbed DOC from labile and recalcitrant pools
$F_{\text{BIOIN}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Decomposed DOC flux from labile and recalcitrant pool into biomass pool
$F_D$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Labile and recalcitrant decomposed DOC flux
$F_{\text{Diff}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Flux of DOC transported by diffusion
$F_{\text{PBIO}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	DOC flux originated from biomass carbon pool
$F_{\text{PDPM}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	DOC flux originated from decomposable plant material carbon pool

Symbol	Units	Definition
$F_{P_{HUM}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	DOC flux originated from humus carbon pool
$F_{P_{RPM}}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	DOC flux originated from resistant plant material carbon pool
$F_S(s)$	$\text{kg m}^{-2}$	Soil moisture rate modifier
$F_T(T_{soil})$	K	Soil temperature rate modifier
$F_v(v)$		Fractional coverage of a vegetation type
$f_{dpm}$		Fraction of litter that is decomposable plant material
$K_P$	$\text{day}^{-1}$	Rate constant for DOC production specific to the pool
$K_{DOC}$	days	Basal decomposition rate of dissolved DOC labile and recalcitrant pools
$K_D$	$\text{m}^3 \text{ water kg}^{-1} \text{ soil}$	Distribution coefficient of adsorbed DOC
$A_c$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Litterfall rate
$L_T$	$\text{kg m}^{-2} \text{ day}^{-1}$	Leaching from labile and recalcitrant DOC pools in top soil
$L_S$	$\text{kg m}^{-2} \text{ day}^{-1}$	Leaching from labile and recalcitrant DOC pools in sub soil
$m$		DOC decomposition rate type (labile or recalcitrant)
$R_{BIO}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Respiration from biomass carbon pool
$R_{DPM}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Respiration from decomposable plant material carbon pool
$R_{DOC}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Respiration from labile and recalcitrant DOC pools
$R_{HUM}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Respiration from humus carbon pool
$R_{RPM}$	$\text{kg C m}^{-2} \text{ day}^{-1}$	Respiration from resistant plant material carbon pool
$R_{off_{surf}}$	$\text{kg m}^{-2} \text{ day}^{-1}$	Surface Runoff

Symbol	Units	Definition
$Roff_{sub}$	$\text{kg m}^{-2} \text{ day}^{-1}$	Sub-Surface Runoff
$S_C$	$\text{kg C m}^{-2}$	Soil carbon storage
$T_s$	$\text{kg m}^{-2}$	Soil moisture content
$S_{DOC}$	$\text{kg C m}^{-2}$	Labile and recalcitrant DOC storages
$S_{DOC_{ad}}$	$\text{kg C m}^{-2}$	Adsorbed labile and recalcitrant DOC storages
$\theta_v$	$\text{kg m}^{-3}$	Volumetric Soil moisture content
$\tau_z$	$\text{m}^{-1}$	Decay of Carbon decomposition with depth
$z$	m	Soil depth
$z_0$	m	e-folding depth of carbon content within 1 meter of soil

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Table 3. Data availability for model evaluation at different

Sites	Brasschaat <sup>1</sup>	Carlow <sup>1</sup>	Guandaushi <sup>2</sup>	Hainich <sup>1</sup>	Turkey-point89 <sup>2</sup>
Carbon fluxes					
<i>GPP</i>	2000-2006	2008		2000-2012	2005-2008
<i>NPP</i>	2000			2000-2007	2005-2008
<i>Soil respiration</i>	2000-2006			2000-2007	2005-2008
<i>C content</i>	1995-1998	2006-2009		2000-2007	2004-2006
DOC measurements					
<i>1 year</i>			1999		
<i>1 to 5 years</i>		2006-2009			2004-2005
<i>5 to 10 years</i>	2000-2008			2001-2014	

1. level 1 site 2. Level 2 site

Table 4. Evaluation Level 1-sites characteristics

	Site		
	Brasschaat	Carlow	Hainich
	Characteristics		
<b>Ecosystem</b>	Evergreen forest	Grassland	Deciduous forest
<b>Soil classification</b>	Arenosol	Luvisol	Cambisols
<b>BK (kg m<sup>-3</sup>)</b>	1.4	1.07	1.2
<b>Clay (fraction)</b>	0.034	0.22	0.589
<b>Sand (fraction)</b>	0.8912	0.51	0.031
<b>Silt (fraction)</b>	0.0748	0.27	0.38
	Measurement depth (cm)		
<b>Carbon content</b>	100 <sup>1</sup>	50 <sup>2</sup>	60 <sup>3</sup>
<b>DOC concentration</b>	10,35,75	5,10,20	10-77
	FLUXNET meteorological observations		
<b>Period</b>	1996-2014	2004-2014	2004-2009

1. Janssens et al. 1999 2. Kindler & Siemens 2010 3. Schrumpf et al. 2011

Table 5. The measured (Obs.) vs. the modelled (Mod.) carbon fluxes, SOC concentration and soil DOC concentration at different soil depths in five study sites.

Variables	Level-1						Level-2			
	Brasschaat		Carlow		Hainich		Turkey Point-89		Guandaushi	
	Obs.	Mod.	Obs.	Mod.	Obs.	Mod.	Obs.	Mod.	Obs.	Mod.
<b>Carbon fluxes (<math>\text{g C m}^{-2} \text{yr}^{-1}</math>) and SOC (<math>\text{kg C m}^{-2}</math>)</b>										
<b>GPP</b>	1173±92	867±25	903	1165	1606±102	1455±168	1732±108	1635±63	-	-
<b>NPP</b>	850	596.1	-	-	673±33	833±153	814±51	1013±92	-	-
<b>Soil Res*</b>	411±34	625±54	-	-	883±206	909±66	693±16	1006±142	-	-
<b>SOC</b>	11.47	8.01	2.3	4.17	11.75	8.63	1.85	3.39	-	-
<b>DOC concentration (<math>\text{mg C L}^{-1}</math>)</b>										
<b>10 cm</b>	39±15	28±13	7±3	6±1	9±3	9±2	-	-	-	-
<b>15 cm</b>	-	-	-	-	-	-	-	-	nh: 19±12 sh: 17±12 cf: 8±15	4±1
<b>20 cm</b>	-	-	-	-	6±2	7±2	-	-	-	-
<b>25 cm</b>	-	-	-	-	-	-	15±4.5	16±4	-	-
<b>10-28 cm</b>	-	-	13±4	4±1	-	-	-	-	-	-
<b>30 cm</b>	-	-	-	-	-	-	-	-	nh: 9±7 sh: 15±8 cf: 7±17	3±1
<b>35 cm</b>	29±2	13±9	-	-	-	-	-	-	-	-
<b>75 cm</b>	22±1	6±6	-	-	-	-	-	-	-	-
<b>28 to 77</b>	-	-	5±2	5±0.2	-	-	-	-	-	-
<b>100 cm</b>	-	-	-	-	-	-	2.2±0.2	7.9±2	-	-

\*: soil respiration, nh: Natural Hardwood; sh: Secondary hardwood; cf: Chinese fir

# Representation of dissolved organic carbon in the JULES land surface model (vn4.4\_JULES-DOCM)

## Supporting information

Table S1.  $z_0$  values for each PFT

PFT	$z_0$
Boreal forest	0.775625
Crops	1.13717
Deserts	1.67113
Sclerophyllous shrubs	1.22839
Temperate deciduous forest	0.725914
Temperate evergreen forest	0.857235
Temperate grassland	1.22839
Tropical deciduous forest	1.67113
Tropical evergreen forest	1.0188
Temperate grassland/savana	1.45185
Tundra	0.656898

Table S2.  $z_0$  values for each PFT in JULES-DOCM

JULES PFT	$z_0$
Tropical broadleaf evergreen forest	1.0188
Temperate broadleaf evergreen forest	0.857235
broadleaf deciduous forest	0.725914
needle-leaf evergreen forest	0.857235
needle-leaf deciduous forest	0.725914
C3 grass	1.13717
C4 grass	1.13717
Evergreen shrubs	1.22839
Deciduous shrubs	1.22839



Table S3. Anova test results for Carbon fluxes (Df: Degree of freedom, Sum sq: sum of squares, Mean sq: mean of squares, Pr: p-value)

ANOVA					
	Df	Sum sq	Mean Sq	F value	Pr(>F)
GPP					
Hainich	1	102955	102955	5.352	0.0343
	16	307785	19237		
Brasschaat	1	280924	280924	62.27	1.33E-05
	10	45117	4512		
Turkey Point-89	1	9295	9295	4.714	0.162
	2	3943	1972		
NPP					
Hainich	1	88254	88254	7.222	0.0362
	6	73323	12220		
Turkey Point-89	1	39632	39632	7.154	0.116
	2	11080	5530		
SOIL RESPIRATION					
Hainich	1	1400	1400	0.06	0.815
	6	140896	23483		
Brasschaat	1	160497	160947	77.44	1.40E-06
	12	24870	2073		
Turkey Point-89	1	98114	98114	9.687	0.0896
	2	20256	10128		

We include all the sensitivity runs for Level-1 sites: Hainich, Brasschaat and Carlow for all the depths where the measurements were available. Red points are indicating measurements where black points are values from model (Fig. S2). Also representing Level-2 sites: Turkey Point 89 and Guandaushi comparison of modelled DOC versus measured in deeper soil depths (Fig. S3).

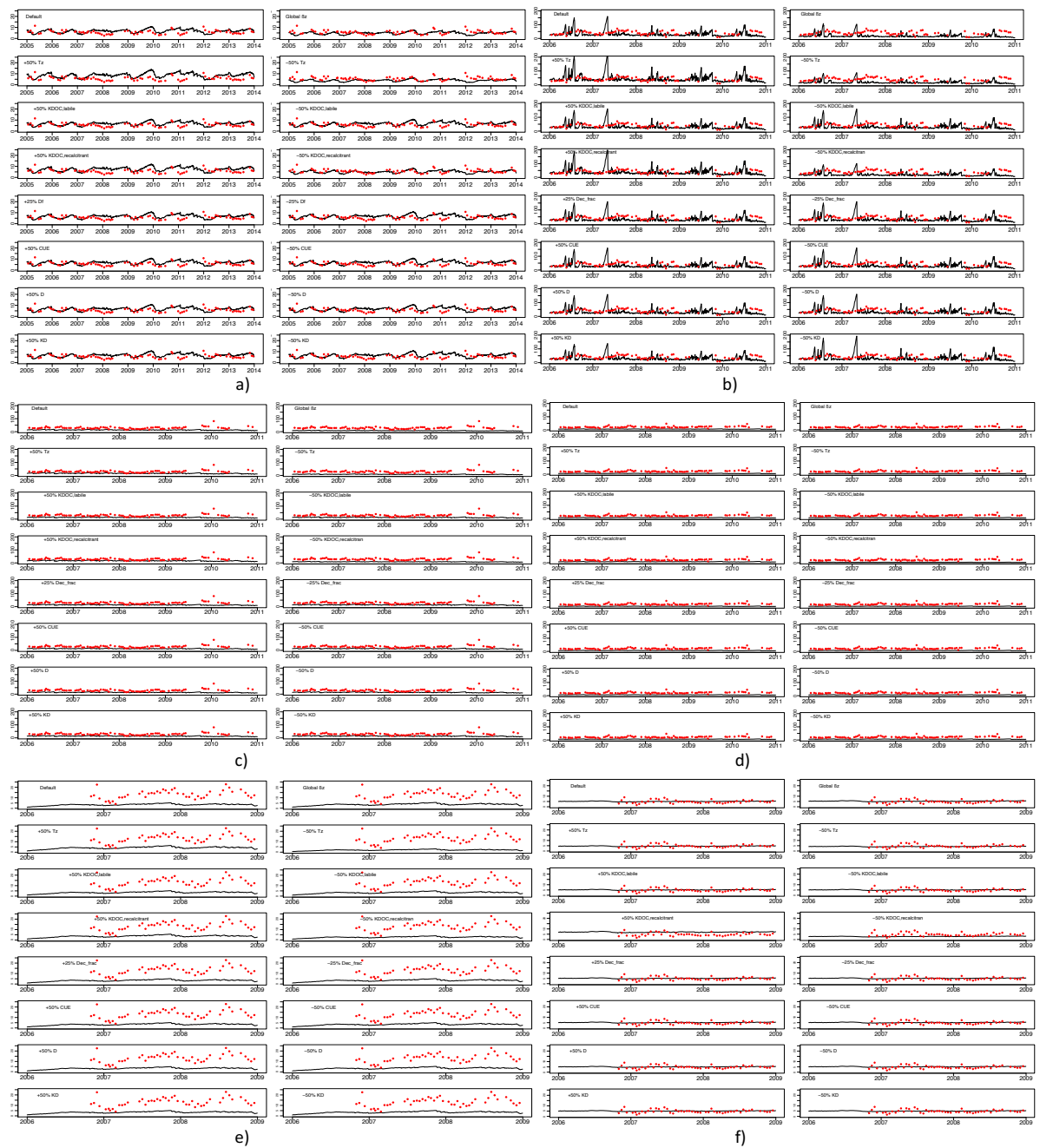


Figure S1. Sensitivity tests (black line) versus measurements (red dot) at a) 20cm depth – 2004-2013, Hainich b) 10cm depth – 2006-2010, Brasschaat c) 35cm depth – 2006-2010, Brasschaat d) 75cm depth – 2006-2010, Brasschaat e) 10 to 28cm depth – 2006-2009, Carlow f) 28 to 78cm depth – 2006-2009, Carlow; X axis is year and Y axis is DOC concentration in  $\text{mg C L}^{-1}$ . Parameter sets description and values in Table 1

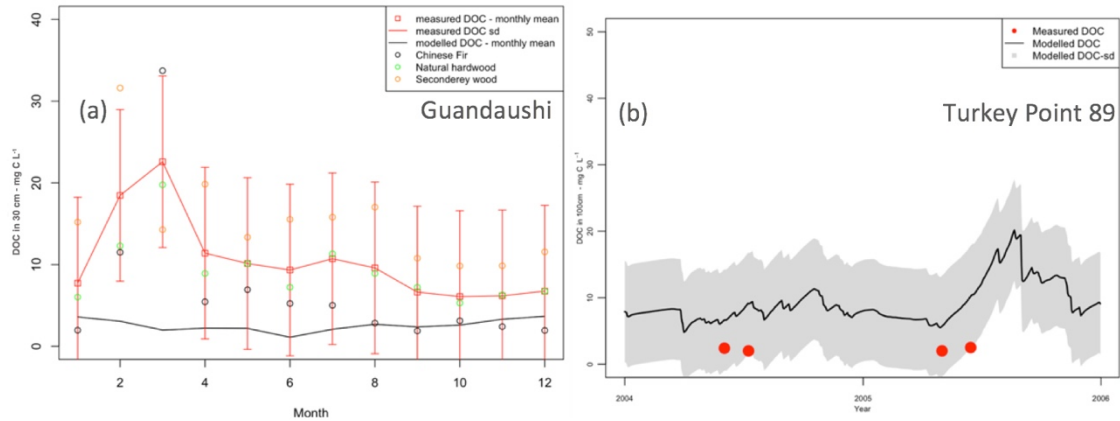


Figure S2. DOC concentration (mg C L<sup>-1</sup>) for (a) Guandaushi at 30 cm measured (black dot: Chinese Fir, green dot: natural hardwood, orange dot: secondary wood, red square: mean, red line: standard deviation) and simulated (black lines) and for (b) Turkey Point 89 at 100 cm measured (red dots) and simulated (black lines, grey line: standard deviation).

We examine the hydrology of the model and its interaction with DOC concentration and leaching for Level-1 sites: Carlow and Brasschat (Fig. S3) and overall model performance in DOC representation in all depths by comparing modelled versus measurements during study period in Hainich, Brasschaat and Carlow (Fig. S4).

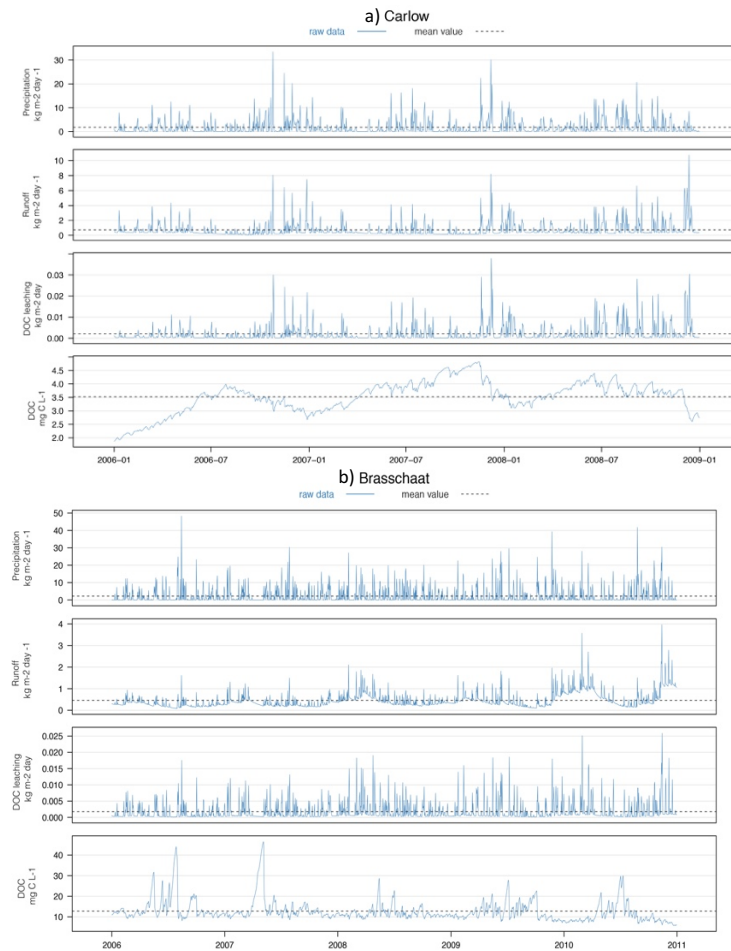


Figure S3. a) Precipitation, runoff, DOC leaching and DOC concentration (down to 3 m averaged) in Carlow from 2006 to 2009 b) in Brasschaat from 2006 to 2010 simulated data with JULES-DOCM

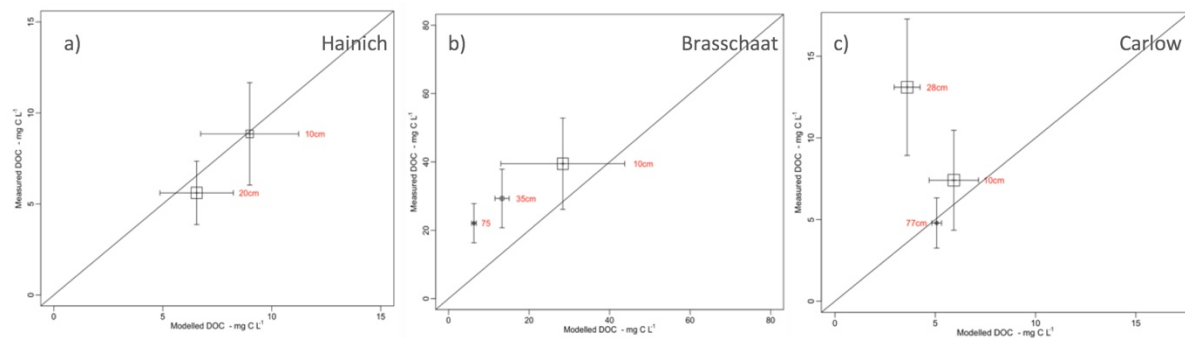


Figure S4. a) Measured vs modelled DOC (mg C L<sup>-1</sup>) with default set in Hainich from 2006 to 2013 at 10 and 20cm b) in Brasschaat from 2006 to 2010 at 10,35 and 75cm c) in Carlow from 2006 to 2009 at 10,10 to 28 and 28 to 78cm

Sensitivity of model parameters (Table S4) was tested in Level-1 Sites for the depths where the DOC measurements were available (Fig. S5) and the results were reported in percentage of change compared to default parameters set (Table S5). Anova test was used in order to determine each parameter's impact significance on DOC representation (Table S6).

Table S4. JULES-DOCM parameters set for sensitivity test

<i>ID</i>	<i>Description</i>
<i>SET-1</i>	<i>PFT based <math>z_0</math></i>
<i>SET-2</i>	<i>Global <math>z_0</math></i>
<i>SET-3</i>	<i>+50% <math>\tau_z</math></i>
<i>SET-4</i>	<i>-50% <math>\tau_z</math></i>
<i>SET-5</i>	<i>+50% <math>K_{DOC, labile}</math></i>
<i>SET-6</i>	<i>-50% <math>K_{DOC, labile}</math></i>
<i>SET-7</i>	<i>+50% <math>K_{DOC, recalcitrant}</math></i>
<i>SET-8</i>	<i>-50% <math>K_{DOC, recalcitrant}</math></i>
<i>SET-9</i>	<i>+25% <math>D_f</math></i>
<i>SET-10</i>	<i>-25% <math>D_f</math></i>
<i>SET-11</i>	<i>+50% <math>CUE</math></i>
<i>SET-12</i>	<i>-50% <math>CUE</math></i>
<i>SET-13</i>	<i>+50% <math>D</math></i>
<i>SET-14</i>	<i>-50% <math>D</math></i>
<i>SET-15</i>	<i>+50% <math>K_D</math></i>
<i>SET-16</i>	<i>-50% <math>K_D</math></i>

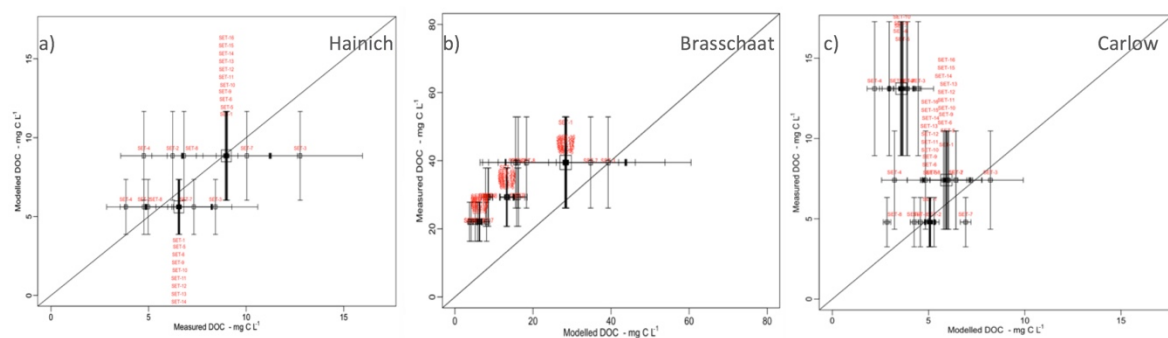


Figure S5. a) Measured (X axis) vs modelled (Y axis) DOC sensitivity runs (Table1) in Hainich from 2006 to 2013 at 10 and 20cm b) in Brasschaat from 2006 to 2010 at 10,35 and 75cm c) in Carlow from 2006 to 2009 at 10,10 to 28 and 28 to 78cm

Table S5. Relative change in simulated DOC (%) for a +50% and -50% changes in model parameters for Hainich, Carlow and Brasschaat

HAINICH		$Z_0$	$\tau_Z$	$K_{\text{DOC-LABILE}}$	$K_{\text{DOC-RECALCITRANT}}$	$D_F$	CUE	D	$K_D$
50%	-	-	24.82748	0.2746118	18.51532	-0.590175	-0.06117	-0.04519973	-0.05364935
	(PFT based $z_0$ )								
-50%	-25.12175	-	-0.2729602	-29.18424	0.586697	0.06068464	0.04545651	0.05483722	
	(global $z_0$ )	36.45213							
CARLOW									
50%	-	16.81662	0.9795210	18.77268	-0.2522954	-0.08957044	0.1873639	-0.05575369	
	(PFT based $z_0$ )								
-50%	6.52764	-31.50205	-0.9754175	-27.40512	0.2517171	0.08983245	-0.2774403	0.05659863	
	(global $z_0$ )								
BRASSCHAAT									
50%	-	27.52056	0.5294166	23.45682	-0.1300973	-0.1176923	-0.3806475	-1.256365	
	(PFT based $z_0$ )								
-50%	-40.6144	-38.92471	-0.5120930	-36.20752	0.1305755	0.1183834	0.3794148	1.571266	
	(global $z_0$ )								



Table S6. Anova test results for sensitivity test of Level-1 sites

ANOVA						ANOVA						ANOVA					
DOC	Df	Sum sq	Mean Sq	F value	Pr(>F)	DOC	Df	Sum sq	Mean Sq	F value	Pr(>F)	DOC	Df	Sum sq	Mean Sq	F value	Pr(>F)
Hainich						Carlow						Brasschaat					
set-2	1	10686	10686	1066	<b>2.00E-16</b>	set-2	1	116	115.98	20.27	<b>6.81E-06</b>	set-2	1	98664	98664	5924	<b>2.00E-16</b>
set-3	1	10437	10437	491.9	<b>2.00E-16</b>	set-3	1	770	769.7	109.73	<b>2.00E-16</b>	set-3	1	45301	45301	126.7	<b>2.00E-16</b>
set-4	1	22499	22499	2572	<b>2.00E-16</b>	set-4	1	2701	2701.1	703.7	<b>2.00E-16</b>	set-4	1	90625	90625	585.2	<b>2.00E-16</b>
set-5	1	1	1.277	0.094	0.759	set-5	1	3	2.611	0.486	0.486	set-5	1	17	16.76	0.069	0.792
set-6	1	1	1.267	0.093	0.76	set-6	1	3	2.59	0.49	0.484	set-6	1	16	15.69	0.065	0.798
set-7	1	5805	5805	382.7	<b>2.00E-16</b>	set-7	1	959	959.2	145.6	<b>2.00E-16</b>	set-7	1	32911	32911	109.1	<b>2.00E-16</b>
set-8	1	14422	14422	1322	<b>2.00E-16</b>	set-8	1	2044	2044.2	488.3	<b>2.00E-16</b>	set-8	1	78414	78414	462.8	<b>2.00E-16</b>
set-9	1	6	5.898	0.437	0.508	set-9	1	0	0.173	0.033	0.857	set-9	1	1	1.01	0.004	0.948
set10	1	6	5.828	0.427	0.514	set10	1	0	0.172	0.032	0.857	set10	1	1	1.02	0.004	0.948
set11	1	0	0.063	0.005	0.946	set11	1	0	0.022	0.004	0.949	set11	1	1	0.83	0.003	0.953
set12	1	0	0.062	0.005	0.946	set12	1	0	0.022	0.004	0.949	set12	1	1	0.83	0.003	0.953
set13	1	0	0.035	0.003	0.96	set13	1	0	0.096	0.018	0.894	set13	1	9	8.67	0.036	0.849
set14	1	0	0.035	0.003	0.96	set14	1	0	0.096	0.018	0.894	set14	1	9	8.61	0.036	0.85
set15	1	0	0.049	0.004	0.952	set15	1	0	0.008	0.002	0.968	set15	1	94	94.41	0.415	0.519
set16	1	0	0.049	0.004	0.952	set16	1	0	0.008	0.002	0.968	set16	1	148	147.7	0.566	0.452

Seasonality of DOC concentration in different depths of Level-1 sites (Hainich, Carlow and Brasschaat) was tested by comparing monthly modelled DOC means versus measurements (Fig. S6).

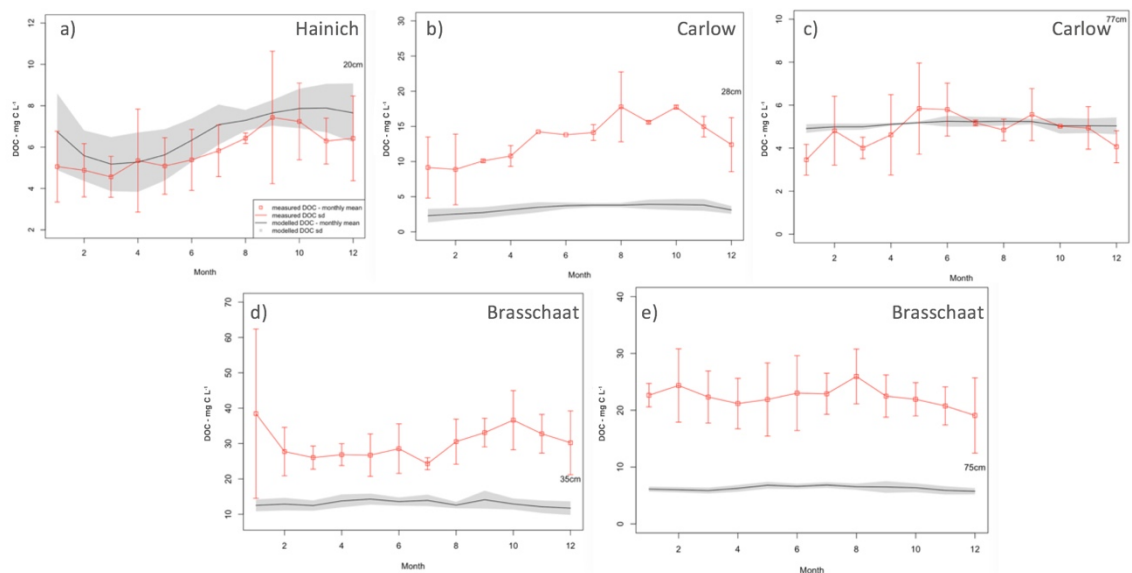


Figure S6. Monthly DOC means modelled versus measured (mg C L<sup>-1</sup>) for studied period at a) 20cm of Hainich b) 10 to 28cm of Carlow c) 28 to 77 cm of Carlow d) 35cm of Brasschaat e) 75cm of Brasschaat