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Sensitivity analysis and calibration of a soil carbon model (SoilGen2) in two contrasting loess forest soils

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Abstract

To accurately estimate past terrestrial carbon pools is the key to understand the global carbon cycle and its relationship with the climate system. SoilGen2 is a useful tool to obtain aspects of soil properties (including carbon content) by simulating soil formation processes; thus it offers an opportunity for past soil carbon pool reconstruction. In or-5 der to apply it to various environmental conditions, parameters related to carbon cycle process in SoilGen2 are calibrated based on 6 soil pedons from two typical loess deposition regions (Belgium and China). Sensitivity analysis using Morris' method shows that decomposition rate of humus (k_{HUM}), fraction of incoming plant material as leaf litter (f_{recto}) and decomposition rate of resistant plant material (k_{RPM}) are 3 most sensi-10 tive parameters that would cause the greatest uncertainty in simulated change of soil organic carbon in both regions. According to the principle of minimizing the difference between simulated and measured organic carbon by comparing quality indices, the suited values of k_{HUM} , fr_{ecto} and k_{BPM} in the model are deduced step by step. The difference of calibrated parameters between Belgium and China may be attributed to their 15 different vegetation types and climate conditions. This calibrated model is improved for better simulation of carbon change in the whole pedon and has potential for future modeling of carbon cycle in paleosols.

1 Introduction

- ²⁰ The terrestrial ecosystem is one of the essential parts of the global carbon cycle. Significant variations of terrestrial carbon pool at geological timescales have played important role in past atmospheric CO₂ concentration change (Falkowski et al., 2000; Post et al., 1990). The soil carbon pool is much larger than the biotic pool (Lal, 2004) and accounts for about 2/3 of the terrestrial carbon pool, thus quantitative estimation of acid carbon pool is the key to reveal the mechanism of past terrestrial carbon evel
- of soil carbon pool is the key to reveal the mechanism of past terrestrial carbon cycle and narrow the uncertainties in the global carbon cycle inventory. However, due to only



parts of carbon pool remaining in sediments, past soil carbon pool reconstruction is difficult by direct measurement. Modeling approaches become the potential option for accurate estimation.

- Currently, with the development of soil carbon models, quantitative simulation of soil carbon storage have been widely done, but most of them focus on modern processes (Coleman et al., 1997; Jensen et al., 1997; Kelly et al., 1997; Li et al., 1997). The simulations on past soil carbon pool are still rare (Finke, 2012; Finke and Hutson, 2008; Mermut et al., 2000), because changes of it at long timescale were the result of soil formation and development processes, the unavailability of information on past soil formation factors for different regions induces uncertainty in estimation (Finke, 2012; Sauer et al., 2012). Furthermore, fewer models could consider soil formation factors
- (Jenny, 1961: e.g. climate, organisms, relief, parent material and time, "CLORPT") in simulation at the same time (Minasny and McBratney, 1999, 2001; Minasny et al., 2008; Parton et al., 1987).
- ¹⁵ SoilGen2 developed by Finke (Finke, 2012; Finke and Hutson, 2008) is a first attempt to reconstruct most aspects of soil evolution by taking all soil formation factors into account. The advantage of the model is that it could simulate organic and inorganic carbon cycle simultaneously and reveal the influences on carbon pool by other soil processes at long time scale. The model has been validated and applied in European
- soils developed from loess parent materials since 15 000 yr ago (Finke, 2012; Finke and Hutson, 2008), and the results show that clear sensitivity and plausible response of this model to the "climate", "organisms" and "relief" factors of soil formation are existed. It also has been confirmed that reconstructions of realistic initial status of soil profiles (including carbon and other elements contents) can be evaluated through simulating with the sense of the sense of the sense.
- ²⁵ soil formation process by SoilGen2 (Sauer et al., 2012). Therefore, the model offers an opportunity to reconstruct the past soil carbon cycle.

Because the verification and application of SoilGen2 is still at its preliminary stage, only parts of the soil processes included in the model have been calibrated (e.g. calcite leaching and clay migration) (Finke, 2012; Finke and Hutson, 2008). No calibration





on parameters related to organic carbon (OC) cycle has been done yet. This work is necessary, and this activity should be preceded by an analysis of such model to determine its most sensitive parameters (Skjemstad et al., 2004). The calibrated model will be the base for soil carbon pool reconstruction in past situations (e.g. via study of paleosols).

In this study, soil pedons from two typical loess deposition regions (Belgium and China) with distinct climate conditions, are selected to calibrate OC cycle process in SoilGen2, because in loess deposits paleosols are found which record detail information of past soil formation. They have been continuously and widely deposited in Eurasia since 22 Myr ago (Guo et al., 2002; Kukla, 1987; Liu, 1985). More than 400

paleosols were developed in the loess-soil sequences in China (Guo et al., 2002), these provide the best record for reconstruction of past carbon cycle through modeling soil formation processes in future studies.

In summary, the objectives of this study are: (1) to use sensitivity analysis to assess which parameters in SoilGen2 potentially cause the greatest uncertainty in calculated change in soil OC in Belgium and China; (2) to calibrate the parameters related to OC cycle in Belgian and Chinese soil pedons. We focus on forest vegetations on loess soils in this study.

2 Material and methods

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20 2.1 Modeling soil carbon change with SoilGen2

SoilGen2 simulates various aspects of pedogenesis including e.g. organic matter (OM) accumulation, clay migration and $CaCO_3$ leaching. In essence, it is an extended solute transport model solving the Richards' equation for unsaturated water flow and the Convection-Dispersion equation for solute transport. Additionally, heat flow is calcu-

²⁵ lated to estimate soil temperature, which allows to evaluate the effect of soil temperature change on values of chemical constants, mineralization of OM and to simulate the



effect of frozen soils on water flow. For detailed model description, reference is made to Finke and Hutson (2008). This article focuses on the description of the OC cycle in SoilGen2, which interacts with other soil formation processes through flow of CO_2 .

Vegetation provides dead plant material (leaf and root litter) as model input (Fig. 1),
which contains Ca²⁺, Mg²⁺, K⁺, Na⁺, Al³⁺, Cl⁻, SO₄²⁻, HCO₃⁻ and CO₃²⁻ previously taken up from the soil solution via the transpiration stream. These ions are following the carbon decomposition pathway described hereunder dependent on vegetation types. 4 vegetation types (grass/scrub, conifers, deciduous wood and agriculture/barley) are identified in SoilGen2 which have each a unique root distribution pattern, associated water ion-uptake and target ion composition in living biomass (Finke, 2012: Table 2). Decomposition rates are considered invariant with respect to the various ion species, which is a simplification of the true system.

Dead plant material is distributed over root and leaf litter with a vegetation-dependent fraction fr_{ecto}, and the root litter input is distributed over the soil depth such that it reflects the root density distribution. These litter inputs are then split and added to the decomposable (DPM) and resistant plant material (RPM) pools using the (vegetationdependent) DPM/RPM factor. These plant material pools, existing in both the ectorganic layer and the individual mineral soil layers (endorganic layer), gradually decompose and mineralize while being incorporated and redistributed in the soil by biotur-

²⁰ bation, which is modeled as an incomplete mixing process (Finke and Hutson, 2008). Each soil layer that is subject to bioturbation contributes a depth-dependent input mass fraction to a bioturbation pool, which is then mixed vertically.

Further decomposition of OM is modeled according to the concepts of the RothC26.3 model (Coleman and Jenkinson, 2005; Jenkinson and Coleman, 1994) using degra-

²⁵ dation rates that are modified as a function of soil temperature and moisture conditions. The mineralization process finally produces CO₂ and releases cations and anions (Finke and Hutson, 2008: Fig. 1) into the soil solution. The decomposition rates of DPM, RPM, biomass (BIO) and humified (HUM) OM are considered similar for all vegetation types. This is also assumed for the scaling factor (scalfac) in the function



that distributes decomposed plant material over mineralized OM, BIO and HUM using the clay content and for the fractionation parameter BIO/HUM.

Figure 1 shows there are 8 parameters that describe the carbon decomposition pathways: fr_{ecto}, DPM/RPM (both for deciduous forest), k_{DPM}, k_{RPM}, scalfac, BIO/HUM,
 *k*_{BIO} and *k*_{HUM}. The relative importance of these parameters will be tested by sensitivity analysis and then calibrated in this study.

2.2 Study regions

2.2.1 Belgian loess soil under permanent deciduous forest

This study concerns soils at 3 topographic positions in the Zonien Forest near Brussels, Belgium (50° 46′ 31″ N, 4° 24′ 9″ E), developed in loess deposited in the Weichselian glaciation. The 3 pedons are located at mutual distances of less than 100 m, but extensive research revealed a clear relation between slope exposition and decalcification depth (Langohr and Sanders, 1985), which was confirmed by model simulations (Finke, 2012). The loess cover is 2–4 m thick and overlies a dissected plateau of pre¹⁵ Weichselian age in tertiary clays that locally cause water stagnation, but not at the 3

- plot sites. Langohr and Saunders (1985) proved that the landscape was hardly eroded in the last 20000 yr. Annals of landowners from the 14th century onwards indicate that this area was never under agriculture, as it was used for hunting by the nobility at least from this time onwards. Older reports indicate that it was a mixed beech-oak forest
- ²⁰ previously. Currently, the area is under beech forest (*Fagus Sylvatica*) with selective felling activity. There is little undergrowth of blackberry (*Rubus fruticosus*). Detailed investigations also showed no evidence of plowing in the soil profiles (Van Ranst, 1981). Thus, soil development shows little human influence. The 3 pedons were classified as (IUSS Working Group WRB, 2006):
- 25 (1) Plateau position: stagnic cutanic fragic Albeluvisol (dystric, greyic, siltic);
 - (2) South facing slope of 12°: cutanic fragic Albeluvisol (dystric, siltic);



(3) North facing slope of 12°: cutanic fragic Albeluvisol (siltic).

Detailed analysis of the mineral soils of these pedons was reported in Finke (2012, Table 3). For this study, samples from the ectorganic litter layers were also taken and analyzed (Table 1) for later comparison with simulation results. Volume and dry weight were measured for bulk density estimation. The weight loss-on-ignition method was used to determine OC.

2.2.2 Chinese loess soil under secondary and artificial deciduous forest

This study concerns other 3 pedons at plateau position located in Ziwu Mountains (35–36° N, 108–110° E), China, which is the best conserved region for secondary natural
 forests on the Loess Plateau. The pedons are developed in the loess deposited since Last Glacial Maximum (LGM). The soil depths are about 1–1.5 m and overlies the older loess deposited in Quaternary. Because Loess Plateau is one of the important culture origin and development centers in China, the vegetation in Ziwu Mountains has been disturbed by human through felling and grazing activities in the Holocene (Liu, 2007).
 However, since 1870s population moved out of the region and in 1970s a forest protection project has been started in this region by Chinese government. Currently, the area is covered with secondary natural forest (e.g. *Quercus liaotungensis, Populus davidiana, Betula platyphylla*) and production forest (e.g. *Robinia*). The 3 pedons' information is as follows:

- LJB (36° 05' N, 108° 34' E) slope of 0°: Luvisol (IUSS Working Group WRB, 2006), secondary natural forest (*Populus davidiana*, 25 yr);
 - 2. ZW_2 (35° 26' N, 108° 33' E) slope of 0°: Kastanozem (IUSS Working Group WRB, 2006), production forest (*Robinia*, 20 yr);
 - 3. ZW₋3 (35° 27′ N, 108° 38′ E) slope of 0°: Kastanozem (IUSS Working Group WRB, 2006), production forest (*Robinia*, 20 yr).



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Samples from ectorganic litter layers were taken in the same way as in Zonien forest of Belgium, while in mineral layers samples were taken at 5–10 cm depth intervals. Bulk densities were measured by volume and dry weight method, and OC contents of them were analyzed by the potassium dichromate method (Table 1).

5 2.3 Model input data

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Two types of inputs are included in SoilGen2, one is for boundary conditions (e.g. climate, litter input and bioturbation history), and another is for initial conditions (e.g. soil properties, typical year weather pattern).

2.3.1 Inputs for Belgium

¹⁰ Climate and weather data were taken from the nearby weather station of Uccle (near Brussels and at 5 km from the studied site). A typical year of daily rainfall and weekly potential evapotranspiration data was used for the whole simulation period with an annual rainfall sum of 849 mm and potential evapotranspiration of 649 mm. The average January temperature was 3 °C and July temperature was 18 °C. An annual litter input of 4.7 Mg C ha⁻¹ yr⁻¹ (personal communication with Arne Verstraeten, Research Institute for Nature and Forest, Belgium) was taken. The bioturbation was assumed to be 8.2 Mg ha⁻¹ yr⁻¹ affecting the upper 30 cm of soil.

Initial physical and chemical properties of the soil pedons were only partly known from measurements (Finke, 2012: Table 3), and to obtain a complete set of initial soil properties we did the following:

(1) Starting from the properties of the C-horizon we simulated soil formation between 15,000 a BP (end of loess deposition) to present. See Finke and Hutson (2008) and Finke (2012) for details concerning the modeling approach and inputs.



(2) The simulated properties at present were taken as initial inputs for the various scenarios of following tests for the sensitivity analysis and calibration. However, simulated OC was re-initialized to 0.5% OC throughout the pedon.

Comparison between simulations and measurements (Finke, 2012: Table 5) showed

that simulations could reproduce the A-E-Bt horizon sequence and also the World Reference Base (WRB) soil classifications based on available (non-morphological) measurements. Therefore these simulations were considered as suitable basis for the current study.

2.3.2 Inputs for China

Representative climate data were interpolated from nearby weather stations in China. The average January/July temperature were -5.89/22.1 °C, -4.77/22.5 °C and -4.70/22.5 °C for LJB, ZW_2 and ZW_3, respectively, while annual rainfall and potential evapotranspiration were 482/1645 mm, 516/1582 mm and 519/1587 mm, based on inverse distance interpolation of 30-yr (1958–1988) monitoring data of 61 weather stations distributed over the Loess Plateau. A typical year of daily rainfall and weekly potential evapotranspiration was from monitoring data of Xifeng in 1978 through comparing the characters of yearly precipitation in 3 weather stations nearby these soil

pedons.

Annual input of litter (Populus 4.5 Mg C ha⁻¹ yr⁻¹, Robinia 4.4 Mg C ha⁻¹ yr⁻¹) was transformed from measured biomass data (including volumes of growing stock per unit area, net annual increments and removals) in ZW forest station (Zhang and Shangguan, 2005), based on the protocol developed by De Wit et al. (2006). The bioturbation was assumed to be 15.3–17.4 Mg ha⁻¹ yr⁻¹ affecting the upper 70 and 100 cm of soil for Populus and Robinia ecosystems, respectively. In addition, distribution of monthly

litter input and roots were adjusted in the model according to observed data of Populus and Robinia ecosystems in Loess Plateau (Cao et al., 2006; Cui et al., 2003; Hu et al., 2010; Zhang et al., 2001).



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Initial physical and chemical properties of the soil pedons were from measurements of their parent material layers at the bottom of pedon (Table 1).

As tests showed that amounts of OC in soil pedons would become stable after 300 years' simulation in case of invariant climate and vegetation conditions (Finke and Hutson, 2008), all the tests in this study have a temporal extent of 1000 yr so that effects of initial values of OC are eliminated.

2.4 Sensitivity analysis method

Sensitivity analysis (SA) determines the response of selected model outputs to variations (within plausible bounds) of uncertain input parameters (Saltelli et al., 2000).

- Results of SA can be used to select and rank the most important parameters for calibration. Various SA methods have been developed (Saltelli et al., 2005). A choice of a particular method is based on a function of the number of parameters to be evaluated and the CPU-time per run. The number of parameters to be evaluated in the current study is 8, and a typical SoilGen-run for a 1000 yr period takes about 20 h CPU time.
- ¹⁵ Under these circumstances, Saltelli et al. (2005) proposed 4 methods: Bayesian Sensitivity Analysis (Oakley et al., 2004), Fractional Factorial Designs (Campolongo et al., 2000), Automated Differentiation techniques (Grievank and Walter, 2008) and Morris' method (Morris, 1991).

Bayesian sensitivity analysis is more efficient than traditional Monte Carlo techniques
 but still requires substantial amounts of simulations and reprogramming of the SoilGen code. This technique is therefore considered beyond the scope of this study. Fractional factorial designs have the disadvantage that assumptions need be made on model behavior. Automated differentiation techniques also require substantial reprogramming of the model code and may lead to results only representing local areas in parameter
 space (Saltelli et al., 2005). Morris' method is feasible in terms of computing time be-

25 space (Saltelli et al., 2005). Morns method is leasible in terms of computing time because it takes samples from levels rather than from distributions of parameters (which may be a drawback when such distributions would be known, but this is not the case here). For the above reasons we chose to apply the latter method.



Morris' method is based on the principle that one factor (model parameter) is varied at a time over a certain number of levels in parameter space. Each variation, comprising 2 simulations, leads to a so-called elementary effect u_i :

$$u_{i} = \frac{Y(x_{1}, x_{2}, \dots, x_{i} + \Delta x_{i}, \dots, x_{k}) - Y(x_{1}, x_{2}, \dots, x_{i}, \dots, x_{k})}{\Delta x_{i}}$$
(1)

- ⁵ where *x* is the parameter value, Δ*x_i* is its imposed variation for factor *i* only (Δ*x_i* = 0 for the other factors) and *Y*(*x*) is the model result with parameter set *x*. Values for *x* are randomly chosen inside a plausible parameter value range [*x_{i,lo}*, *x_{i,hi}* Δ*x_i*], and Δ*x_i* is either 0 or a predetermined multiple of 1/(*p* 1) with *p* the number of considered parameter levels (rescaled at range [0;1]). In this study we took *p* = 8, and fixed Δ*x_i* at 2 × 1/(8 1) on the [0, 1] rescaled range. The obtained elementary effects *u_i* comprise a simple random sample, of which the mean μ_i and standard deviation σ_i are used to assess how important a factor is. Hereto, a graph is made displaying the position of a factor *i* in terms of μ_i^{*} (the average of |*u_i*|) and σ_i. If the value of μ_i^{*} is high then there is a high linear effect of factor *i*; large values of σ_i indicate either non-linear behavior
 ¹⁵ In this study we took p = a parameter values).
- In this study we took 8 parameter levels, resulting in 4 elementary effects, for each one of 8 model parameters. Thus, 64 simulations (32 pairs) for a period of 1000 yr were done for a typical loess forest soil in Belgium (2.5 m depth with a vertical discretization of 5 cm at the Uccle Plateau location) and 64 more for a loess forest soil in China
- (1.5 m depth with the same vertical discretization at pedon of LJB). This comprised about 85 CPU-days simulation time on 1 core (less than 6 days on 4 quad core PC's), which was considered feasible. The model output parameters considered were OC (tha⁻¹) in ectorganic layers and OC (mass tha⁻¹ and content %) in the mineral soil. Separate analyses were done for ectorganic layers and endorganic layers because later collibration would focus on the vertical distribution of OC.
- ²⁵ later calibration would focus on the vertical distribution of OC.



2.5 Calibration approach

Calibration is the process of modifying the input parameters to a model until the output from the model matches an observed set of data. Various techniques also have been developed for model calibration, which differ in how parameter combinations are

- ⁵ generated and how results are compared. In many cases, the modeler selects parameter combinations and evaluates results by expert judgment, in which case calibration is more or less a skill and may not detect the optimal parameter combinations. An alternative, often used technique is the minimization of an object function describing the deviations between measurements and simulations for various settings of parame-
- ters. The minimization process advises on optimal parameter combinations under the assumption that model outputs are differentiable with respect to the model parameters.

A well-known implementation is the PEST-software (Doherty, 2004). Model runs are sequential and the software decides if a new run with changed parameter settings is needed after results of a preceding run have been confronted to measurements

- ¹⁵ by evaluating the object function. Another emerging method is the exploration of parameter space by a Markov Chain Monte Carlo Method. Model results are evaluated by calculating the posterior probability of the parameter set given the data, using the prior distribution of the parameters and a likelihood that expresses the correspondence between measurements and simulations. Of this Bayesian calibration method various
- implementations exist, but even the most efficient ones (Vrugt et al., 2009) require numerous simulations. With time consuming models such as SoilGen convergence may take very long both in PEST and in Bayesian calibration. Finke (2012) used therefore an alternative approach in which various chosen sets of parameters were run with the model in parallel, confronting the model with measured data to quantify simulation ac-
- ²⁵ curacy and fitting a polynomial function predicting simulation accuracy as a function of parameter value. Analyzing the partial derivatives of this function the position in parameter space with optimal simulation results was predicted. This approach may not





find the true optimal parameter set and also depends on the choice of the evaluated parameter values, however, for reasons of runtime it was applied in Finke (2012).

The overall procedure of calibration is given in Fig. 2 in the principle of minimizing the difference between measured and simulated OC step by step. During the steps,

- parallel tests were firstly done for soil pedons by varying the most sensitive parameters 5 identified in sensitive analysis. Then the results were evaluated according to the quality indices described below. If there was still possibility to reduce the difference between measured and simulated OC by varying the same parameter, more parallel tests would be done under a sub-range of the parameter; otherwise, inferior next, less sensitive,
- parameter would be selected for tests. The process would be repeated, according to 10 the order of parameters' sensitivity, until no improvement was identified. In both studied regions, the difference of simulated and measured total carbon of the whole pedon was firstly minimized. In the next step, the distribution of OC over ectorganic and endorganic layers was calibrated. The variation range of above parameters would be roughly set according to the guantitative relationships between changed OC and themselves as 15
- previously revealed by sensitivity analysis.

The indices used for assessing the quality of the C-module of SoilGen2 are:

1. Root mean square deviation (RMSE) of total simulated and measured OC mass per mineral soil compartment:

$$RMSE1_{endo,pedon} = \sqrt{\frac{\sum_{k=1}^{K} \left(\left(f_{OC\,M\,k} \times \rho_{M\,k} \times T_k \right) - \left(f_{OC\,Sk} \times \rho_{Sk} \times T_k \right) \right)^2}{K}}$$
(2)

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where $f_{\rm OCM}$ and $f_{\rm OCS}$ are measured and simulated OC mass, respectively, $\rho_{\rm M}$ and $\rho_{\rm S}$ are measured and simulated bulk density (kg dm⁻³), T is the thickness of the k soil compartments (all equal to 50 mm). RMSE1_{endo,pedon} of the 3 pedons in each region are averaged to obtain RMSE1_{endo}.



2. RMSE of total simulated and measured OC mass in the ectorganic layer:

$$\mathsf{RMSE}_{\mathsf{ecto}} = \sqrt{\frac{1}{N} \times \sum_{n=1}^{N} \left(f_{\mathsf{OCM}n} \times \rho_{\mathsf{M}n} \times T_n - \mathsf{OC}_{\mathsf{S}n} \right)^2}$$
(3)

where OC_S is the simulated OC mass in ectorganic layers and *n* is the number of pedons (3 per region).

5 3. RMSE of total simulated and measured OC mass in the whole soil pedon:

$$\mathsf{RMSE}_{\mathsf{OCMS}} = \sqrt{\begin{cases} \frac{1}{N} \times \sum_{n=1}^{N} \left(\left(\sum_{k=1}^{K} \left(f_{\mathsf{OCM}k,n} \times \rho_{\mathsf{M}k,n} \times T_{k,n} \right) + f_{\mathsf{OCM}n} \times \rho_{\mathsf{M}n} \times T_{n} \right) \\ - \left(\sum_{k=1}^{K} \left(f_{\mathsf{OCS}k,n} \times \rho_{\mathsf{S}k,n} \times T_{k,n} \right) + \mathsf{OC}_{\mathsf{S}n} \right) \end{cases}^{2} \end{cases}}$$

$$(4)$$

4. Mean Difference (MD) of total simulated and measured OC mass in mineral soil:

$$\mathsf{MD}_{\mathsf{endo}} = \frac{1}{N} \times \sum_{n=1}^{N} \sum_{k=1}^{K} \left(f_{\mathsf{OCM}\,k,n} \times \rho_{\mathsf{M}\,k,n} \times T_{k,n} \right) - \sum_{k=1}^{K} \left(f_{\mathsf{OCS}\,k,n} \times \rho_{\mathsf{S}\,k,n} \times T_{k,n} \right)$$
(5)

5. Mean Difference of total simulated and measured OC mass in ectorganic layers:

$$MD_{ecto} = \frac{1}{N} \times \sum_{n=1}^{N} (f_{OCMn} \times \rho_{Mn} \times T_n - OC_{Sn})$$
(6)

6. Mean Difference of total simulated and measured OC mass in the whole soil pedon:

$$MD_{OCMS} = MD_{endo} + MD_{ecto}$$

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(7)

7. RMSE of simulated and measured OC % in mineral soil:

$$\mathsf{RMSE2}_{\mathsf{endo},\mathsf{pedon}} = \sqrt{\frac{\sum_{k=1}^{K} \left(\left(f_{\mathsf{OCM}\,k} \times 100 \right) - \left(f_{\mathsf{OCS}\,k} \times 100 \right) \right)^2}{K}}$$

which is averaged over 3 pedons to obtain RMSE2_{endo}.

8. Dissimilarity (DIS) (Gower, 1971) of simulated and measured OC% in mineral soil:

$$DIS_{pedon} = \frac{1}{K \times (OC\%_{max} - OC\%_{min})} \times \sum_{k=1}^{K} abs(f_{OCM\,k} \times 100 - f_{OCS\,k} \times 100) \quad (9)$$

where OC $\%_{max}$ and OC $\%_{min}$ are the maximal and minimal value found in a particular pedon. $\text{DIS}_{OC\%}$ is calculated by averaging over 3 pedons and varies between 0 (perfect) and 1 (very poor).

¹⁰ Of these statistics, the first 6 express how well the total OC mass in the soil is simulated, while the last 2 express how well the vertical distribution of OC content over the pedon is simulated.

3 Results and discussion

3.1 Sensitivity analysis

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¹⁵ Table 2 gives the model parameters that were considered in the sensitivity analysis and the plausible range of these parameters. Figure 3 at a double-logarithmic scale the μ^* and σ of the elementary effects of the 8 factors are shown. The μ for all rate factors were negative, which was expected because these describe decomposition



(8)

and positive values for Δx_i , leading to higher values for *k*, are expected to lead to lower amounts of remaining OC.

The OC mass in ectorganic layers and endorganic layers as well as the OC % in endorganic layers respond most sensitively to the decomposition rate of humus k_{HUM} and less sensitive to the fraction of dead plant material entering the soil as leaf litter fr_{ecto}, k_{RPM} , and scalfac. The other factors show less sensitivity. Most responses are between the |u| = SEM (stand error of the mean) and $|u| = 2 \times SEM$ lines indicating a fair confidence level. Most certain response of the sensitive factors is that of fr_{ecto} while the other factors are less certain. This may be caused by non-linear response or non-additive behavior (the model responds to interactions of factors).

The sensitivity order in the ectorganic layer is similar to that of the mineral soil, except for k_{RPM} and fr_{ecto} . k_{RPM} is more important in the ectorganic layer, the rate modification due to moisture deficit is always equal to 1 in ectorganic layers while it can decrease in the mineral soil (Coleman and Jenkinson, 2005). This results in stronger modified k_{RPM} in the ectorganic layer.

Comparison (Table 2 and Fig. 3) of results for the Chinese and Belgian loess forest soils shows that the sensitivity order of the factors follow the same pattern, irrespective of the differences in soil (the Belgian loess soil is strongly leached whereas the Chinese is not) and climate (a large precipitation surplus in Belgium and a large precipitation deficit in China). The values for μ^* and σ differ (Fig. 3), which is higher in endorganic layers in Chinese soil pedons but lower in ectorganic layers. Nevertheless, the sensitivity order is the same, which means that the same model parameters could be selected for calibration in both soils: k_{HUM} , fr_{ecto}, k_{BPM} and scalfac.

3.2 Calibration

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14 and 8 tests have been done for soil pedons in Belgium and China in 4 and 3 steps, respectively. Table 3 gives the model parameters used in the calibrations in two regions and corresponding steps they belong to. Graphs comparing simulated and measured



OC by 8 quality indices are given in Fig. 4, lower absolute values of these indices indicate better simulated results.

In the first steps of calibration, tests (1b and 1c) with default values of parameters in SoilGen2 show that simulated total OC mass are lower than measured ones in 5 both regions with larger deviation in Belgium (60.08 tha⁻¹) than in China (12.78 tha⁻¹) (Fig. 4c, d).

In the second step, the calibrations were started by increasing total OC masses simulation by decreasing the most sensitive parameter (k_{HUM}) selected based on sensitivity analysis (Table 2). In Belgium, with the decrease of k_{HUM} from 0.014, 0.010 to 0.006,

- the MD_{OCMS} of soil pedons decreased from 47.93, 31.84 to -4.56 tha^{-1} . The moderate value of k_{HUM} (0.010) was chosen as the base for further calibration, because minimizing the difference between simulated and measured OC would be realized step by step with decrease of other parameters.
- In the third step of Belgium, the second sensitive parameter k_{RPM} was varied from ¹⁵ 0.180 to 0.090 by (Test5b–10b). Among these tests, $k_{\text{RPM}} = 0.110$ (Test9b) with secondly lowest RMSE_{OCMS} (10.65 tha⁻¹) and MD_{OCMS} (3.55 tha⁻¹) was preferred, because MD_{OCMS} (-0.91 tha⁻¹) in Test10b has become negative.

In China, the difference between simulated and measured total OC could be minimized by decrease of one parameter k_{HUM} , and also $k_{HUM} = 0.017$ (Test2c) with secondly lowest RMSE_{OCMS} (11.93 tha⁻¹) and MD_{OCMS} (6.42 tha⁻¹) values was used as the base for following steps.

The following calibrations for both regions were to adjust the distribution of OC in ectorganic (overestimation) and endorganic (underestimation) layers. In Belgium, fr_{ecto} was decreased from 0.380 to 0.270, inducing the corresponding decrease of RMSE_{ecto}, RMSE1_{endo}, MD_{ecto} and MD_{endo}, the lowest values of these indices were obtained in Test14b with the following combination of parameters ($k_{HUM} = 0.010$, $k_{RPM} = 0.110$ and $fr_{ecto} = 0.270$). In China, fr_{ecto} was also decreased from 0.480 to 0.380, and the best result was obtained in Test8c ($k_{HUM} = 0.017$, $k_{RPM} = 0.300$ and $fr_{ecto} = 0.400$).

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Test 8c and Test 14b were further confirmed as the best calibration results by comparing 8 quality indices synthetically (Table 3 and Fig. 5), because the indices of them all belong to the first 4 lowest ones in all tests of two regions. Figure 5 further shows that the simulated vertical distributions of OC of them are also similar to measured ones visually.

3.3 Comparison

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3.3.1 Comparison with former studies

Our results of sensitivity analysis are in accordance with former studies on RothC model in surface forest soils (Paul and Polglase, 2004; Paul et al., 2003), which inlicated that change in soil carbon is particularly sensitive to the decomposition rates of HUM, RPM and BIO pools. Comparing that only the relative importance of the parameters was shown in former analysis (Paul and Polglase, 2004; Paul et al., 2003), a quantitative evaluation of their importance is given in our study and the especially significant sensitivity of $k_{\rm HUM}$ is revealed.

¹⁵ The calibrated values of parameters (k_{HUM} and k_{RPM}) in our study all fall into the logical range of former calibrations for RothC model (Shirato et al., 2004; Skjemstad et al., 2004; Todorovic et al., 2010), covering various climate conditions and soil types, They are lower than default values in RothC model, which was originally developed and parameterized in surface agricultural soils (0–30 cm) (Jenkinson, 1990). The dif-

- ference may be attributed to following aspects: firstly, decomposition in agricultural soils is faster than that in forest soils because of its lower lignin content in litter (Lambers et al., 1998) and more favorable micro-climate conditions for decomposition induced by human disturbance (Schlesinger and Andrews, 2000); secondly, carbon at deeper depth (1.5–2.5 m in our study) is older than that near the surface, indicating that it has
- ²⁵ a greater resistance to decomposition or that the environment at depth is less favorable for decomposition processes (Swift, 2001).



The calibrated fr_{ecto} is also lower than default value (0.580) in SoilGen2 from measurement data from literature (Kononova, 1975). Contrary to that part of litter carbon pool in ectorganic layer leaches to endorganic layer by dissolved organic carbon in realistic soil carbon cycle process, the carbon pools in ectorganic and endorganic layers

do little exchange with each other in the simulation of SoilGen2 since ectorganic carbon pools are only limited brought into the mineral soil by bioturbation. Therefore, fr_{ecto}, as the ratio of carbon pool in ectorganic layer to the total pool, would be decreased to offset the influence by leaching.

3.3.2 Comparison between two regions

- ¹⁰ Although the orders of sensitivity for parameters are the same in two regions, the responses are less significant in Belgian soil pedons (Table 2). It led to corresponding larger ranges of parameters (k_{HUM} , fr_{ecto} and k_{RPM}) varied during calibration in Belgium (Table 3), which shows slower decomposition rate of OC in Belgian soils. The differences may be driven by the following reasons.
- Firstly, litter chemical composition is one of the most important factors that affect decomposition of litter. Especially in late stage of decomposition for the formation of humus, lignin decomposition exerts the dominant control in soils (Berg and McClaugherty, 2008; Quideau et al., 2001), which is relative resistant to decomposition (Lambers et al., 1998). Since the study area in Belgium is under beech forest while it is under poplar in China, higher lignin and holocellufose contents in the former ecosystem than the latter (Coldwell and Delong, 1950) induces slower decomposition rate of OC in Bel-
- gium than in China, which is reflected by lower decomposition coefficients (k_{HUM} , fr_{ecto} and k_{RPM}) of resistant carbon pools.

Secondly, the distribution of temperature, precipitation and evaporation over the year
 ²⁵ also affects the decomposition rate and the loss of carbon from soil (Raich and Tufek-cioglu, 2000; Schimel et al., 1994). High temperature accompanying with significant rain occur in summer monsoon climate of China, which could lead quicker litter decomposition (Raich and Tufekcioglu, 2000; Zhang et al., 2008) without any limit of energy



or moisture in this season. The different influences of climate conditions on decomposition process in two regions may be reflected indirectly by setting different values of these parameters, because just decomposition coefficients (k_{HUM} , fr_{ecto} and k_{RPM}) of soil carbon pools were calibrated in this study, and not the mechanisms that mimic the effect of temperature and moisture on decomposition.

4 Conclusions

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Sensitivity analysis based on Morris' method shows that k_{HUM} , fr_{ecto} and k_{RPM} are 3 most important parameters in SoilGen2 to affect change of OC both in Belgian and Chinese soil pedons. The sensitivity orders of the parameters follow the same pattern in two regions but the values of elementary effects differ.

According to the results of sensitivity analysis, SoilGen2 are calibrated by decreasing k_{HUM} , fr_{ecto} and k_{RPM} . The final results are obtained by the following combination of parameters in Belgium ($k_{\text{HUM}} = 0.010$, $k_{\text{RPM}} = 0.110$ and fr_{ecto} = 0.270) and China ($k_{\text{HUM}} = 0.017$, $k_{\text{RPM}} = 0.300$ and fr_{ecto} = 0.400). The less significant sensitive of parameters in sensitivity analysis and larger variation of parameters during calibration in Belgium than in China may be attributed to their distinct vegetation types and climate conditions.

The calibrated parameters follow the law that deeper soil are more resistant to decompose than surface soils induced by the age of carbon and unfavorable environment.

- ²⁰ This indicates that the calibration allows better simulation of carbon storage in the whole soil pedon. With the application of SoilGen2 to loess-soil sequences deposited in China in future studies, quantitative estimates of past soil carbon pools will be reconstructed, which will offer an opportunity to understand the mechanism of carbon cycle at geological timescale.
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Table 1. Selected analytical results of ectorganic and endorganic layers in Belgian and Chinese pedons. Results for endorganic layers of Belgian pedons were published in Finke (2012).

Ectorganic layer								
Region	Pedon	Bulk density	OC					
		(kg dm ⁻³)	(Mg ha ⁻¹)					
Belgium	Plateau	0.090	15.372					
	South facing slope	0.123	24.910					
	North facing slope	0.146	27.142					
China	LJB	0.243	15.432					
	ZW_2	0.226	13.182					
	ZW_3	0.139	12.095					
	Endorganic	: layer						
Depth (cm)		OC (%)						
Pedon	China LJB	China ZW_2	China ZW_3					
0–5	5.058	1.819	2.434					
5–10	4.310	1.888	3.004					
10–15	2.643	2.140	1 752					
15–20	1.594	2.015	1.752					
20–25	1.360	1.831	1 103					
25–30	1.340	1.352	1.155					
30-35	0.959		0.550					
35-40		1.314						
40-45 45-50	0.766		0.801					
40-50 50-55								
55-60		0.927						
60–65	0.521		0.679					
65–70		0.605						
70–75		0.095						
75–80	0.914	0.603	0.596					
80-85		0.000	0.000					
85–90		0.475						
90-95	0.785		0.480					
95-100								
100-105		0.498						
105-110								
110-115								

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Factor	Meaning	Default	Plausible	OC ectorganic (ton ha ⁻¹)		¹)	OC endorganic (ton ha ⁻¹)				OC endorganic (%)				
		value	range	Belgium China		Belgium China			nina	Belgium		China			
				μ^*	σ	μ^*	σ	μ^*	σ	μ^*	σ	μ^*	σ	μ^*	σ
k _{HUM}	Decomposition rate (yr ⁻¹) of Humus	0.02 ^a	0.005-0.035	1569.08	2085.04	630.23	708.39	2218.87	3131.79	4796.81	6064.40	17.85	24.57	35.51	43.51
k _{RPM}	Decomposition rate Plant Material (yr ⁻¹) of Resistant	0.30 ^a	0.075-0.525	120.60	131.04	119.36	129.70	40.41	33.22	80.47	61.18	0.34	0.28	0.61	0.46
fr _{ecto}	Fraction of incoming plant material as leaf litter	0.58 ^b	0.36-0.98	56.21	21.55	38.50	9.17	77.92	35.29	110.43	29.42	0.65	0.29	0.84	0.21
scalfac	Scaling factor for CO ₂ /(BIO+HUM) ratio	1.67 ^a	0.4–3.0	12.81	13.71	8.75	8.77	18.08	23.02	37.78	43.26	0.15	0.19	0.29	0.32
DPM/ RPM	Ratio decompos- able/resistant plant material in incoming plant material	0.25 ^a	0.1–0.5	6.27	1.02	6.21	1.04	4.09	2.16	7.36	3.01	0.03	0.02	0.06	0.02
BIO/ HUM	Distribution ratio of BIO+HUM	0.85 ^a	0.68-1.02	6.93	4.84	5.04	3.30	6.77	2.10	16.86	3.88	0.06	0.02	0.13	0.03
k _{BIO}	Decomposition rate (yr ⁻¹) of Biomass	0.66 ^a	0.165-1.155	1.50	0.81	1.32	0.67	2.39	2.49	3.56	3.01	0.02	0.02	0.03	0.02
k _{DPM}	Decomposition rate (yr ⁻¹) of Decompos- able Plant Material	10.00 ^a	2.5–17.5	0.02	0.01	0.01	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00

Table 2. Model parameters in the organic C-module in SoilGen2 and results of sensitivity analysis.

^a Source: RothC26.3.

^b Source: SoilGen2.17, deciduous woodland.

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Region	Step	Test	Parameters						Quality in	dices			
0	•		$K_{\rm HUM}$	$K_{\rm RPM}$	fr _{ecto}	RMSE _{OCMS}	RMSE _{ecto}	$RMSE1_{endo}$	MD _{OCMS}	MD _{ecto}	MD _{endo}	$RMSE2_{endo}$	DIS_{pedon}
Belgium	1	1b	0.020	0.300	0.580	60.957	5.235	61.536	60.080	-1.164	61.244	0.748	0.236
	2	2b	0.014	0.300	0.580	49.024	7.228	53.382	47.933	-5.117	53.050	0.666	0.211
		Зb	0.010	0.300	0.580	33.442	10.860	41.837	31.838	-9.586	41.424	0.574	0.179
		4b	0.006	0.300	0.580	11.217	18.212	14.209	-4.558	-17.482	12.924	0.525	0.165
	3	5b	0.010	0.180	0.580	40.326	5.460	37.536	39.028	1.939	37.089	0.545	0.169
		6b	0.010	0.135	0.580	15.746	21.984	33.951	12.082	-21.383	33.465	0.523	0.161
		7b	0.010	0.090	0.580	11.770	32.752	26.807	-6.149	-32.352	26.203	0.488	0.154
		8b	0.010	0.120	0.580	12.416	24.917	32.164	7.267	-24.388	31.656	0.513	0.159
		9b	0.010	0.110	0.580	10.653	27.117	30.706	3.545	-26.632	30.177	0.505	0.157
		10b	0.010	0.100	0.580	10.045	29.765	28.972	-0.907	-29.324	28.417	0.497	0.156
	4	11b	0.010	0.110	0.380	10.064	10.960	12.150	1.056	-9.699	10.755	0.442	0.144
		12b	0.010	0.110	0.330	10.031	7.478	8.167	0.414	-5.465	5.879	0.440	0.144
		13b	0.010	0.110	0.280	10.058	5.251	5.776	-0.246	-1.232	0.986	0.445	0.145
		14b	0.010	0.110	0.270	10.070	5.119	5.697	-0.377	-0.385	0.009	0.446	0.145
China	1	1c	0.020	0.300	0.580	16.073	5.977	20.945	12.781	-5.818	18.599	0.677	0.183
	2	2c	0.017	0.300	0.580	11.928	6.530	16.292	6.420	-6.417	12.837	0.648	0.179
		3c	0.014	0.300	0.580	11.002	7.609	11.045	-3.801	-7.505	3.704	0.612	0.174
		4c	0.011	0.300	0.580	22.028	8.968	15.075	-19.233	-8.871	-10.362	0.576	0.170
	3	5c	0.017	0.300	0.480	10.557	3.220	11.720	2.741	-2.971	5.713	0.637	0.180
		6c	0.017	0.300	0.430	10.306	1.770	10.560	0.951	-1.249	2.199	0.634	0.182
		7c	0.017	0.300	0.380	10.368	1.356	10.508	-0.817	0.474	-1.291	0.632	0.184
		8c	0.017	0.300	0.400	10.304	1.283	10.386	-0.110	-0.214	0.104	0.633	0.183

Table 3. Model parameters in the organic C-module in SoilGen2 and quality indices of averageOC of three pedons during the calibration in Belgium and China.

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Fig. 2. Calibration procedure for OC cycle in SoilGen2 and the order of events.





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Fig. 3. Estimated means (μ^*) and standard deviations (σ) of the distribution of elementary effects of factors on OC **(a)** OC mass in ectorganic layers; **(b)** OC mass in endorganic layers; **(c)** OC content in endorganic layers. Closed symbols with names indicate the 4 most important factors.



Fig. 4. Quality indices for calibration results (a) RMSE of average OC mass in three pedons in Belgium; (b) RMSE of average OC mass in three pedons in China; (c) MD of average OC mass in three pedons in Belgium; (d) MD of average OC mass in three pedons in China; (e) RMSE of OC content in three pedons and average values in Belgium; (f) RMSE of OC content in three pedons and average values in China; (g) DIS of OC content in three pedons and average values in Belgium; (h) DIS of OC content in three pedons and average values in China; (g) DIS of OC content in three pedons and average values in China.





Fig. 5. Comparison of vertical distribution of simulated vs. measured OC content in soil pedons (a) Belgium; (b) China. Min are minimal values while Max are maximal values.

