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Inverse determination of heterotrophic soil respiration response to temperature and water content under field conditions

J. Bauer · L. Weihermüller · J. A. Huisman · M. Herbst · A. Graf · J. M. Séquaris · H. Vereecken

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Abstract Heterotrophic soil respiration is an important flux within the global carbon cycle. Exact knowledge of the response functions for soil temperature and soil water content is crucial for a reliable prediction of soil carbon turnover. The classical statistical approach for the in situ determination of the temperature response (Q_{10} or activation energy) of field soil respiration has been criticised for neglecting confounding factors, such as spatial and temporal changes in soil water content and soil organic matter. The aim of this paper is to evaluate an alternative method to estimate the temperature and soil water content response of heterotrophic soil respiration. The new method relies on inverse parameter estimation using a 1-dimensional CO_2 transport and carbon turnover model. Inversion results showed that different formulations of the temperature response function resulted in estimated response factors that hardly deviated over the entire range of soil water content and for temperature below 25°C. For higher temperatures, the temperature response was highly uncertain due to the infrequent occurrence of soil temperatures above 25°C. The temperature sensitivity obtained using inverse modelling was within the range of temperature sensitivities estimated from statistical processing of the data. It was concluded that inverse parameter estimation is a promising tool for the determination of the temperature and soil water content response of soil respiration. Future synthetic model studies should investigate to what extent the inverse modelling approach can disentangle confounding factors that typically affect statistical estimates of the sensitivity of soil respiration to temperature and soil water content.

Keywords Heterotrophic soil respiration · Temperature sensitivity · Soil water content sensitivity · Inverse parameter estimation · SOILCO2/RothC · SCE algorithm · AIC

Introduction

Soil respiration is an important flux of CO_2 to the atmosphere (Schlesinger and Andrews 2000). Against the background of global climate change, reliable model predictions of soil respiration are highly relevant. Among other factors, accurate knowledge of the response of soil carbon decomposition to

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J. Bauer · L. Weihermüller · J. A. Huisman · M. Herbst · A. Graf · J. M. Séquaris · H. Vereecken
Institute of Bio- and Geosciences—Agrosphere, IBG-3, Forschungszentrum Jülich GmbH, Leo Brandt Straße, 52425 Jülich, Germany

J. Bauer (✉)
Institute for Atmospheric and Environmental Sciences, Goethe University Frankfurt am Main, Altenhöferallee 1, 60438 Frankfurt am Main, Germany
e-mail: Bauer@iau.uni-frankfurt.de

changes in soil temperature and water content is essential for reliable predictions (Davidson and Janssens 2006).

Both laboratory and field experiments have been used to determine the response of heterotrophic soil respiration to changes in soil temperature. Laboratory studies are considered to provide more reliable estimates of temperature responses than field experiments (Kirschbaum 2000, 2006). However, laboratory incubation experiments are typically performed under highly artificial conditions. For example, the natural soil structure is commonly destroyed by sieving and homogenisation. Therefore, the transferability of response equations determined in the laboratory to the field is questionable.

The direct estimation of the response of heterotrophic soil respiration to temperature from in situ measurements is complicated and often biased by confounding factors. One important confounding factor is the soil water content. High temperatures are often accompanied by low water contents and vice versa (e.g. Davidson et al. 1998). Such a strong interdependency makes it difficult to separate the effects of temperature and soil water content on soil respiration. Furthermore, changes in soil organic matter (SOM) quantity and quality during the course of a field experiment (e.g. fresh litter input, depletion of labile compounds) could strongly influence the direct estimation of response functions (Larionova et al. 2007; Leifeld and Fuhrer 2005; Mahecha et al. 2010). A third confounding factor is that soil respiration originates from two processes: (i) the decomposition of soil organic matter (heterotrophic respiration) and (ii) root respiration. Both processes probably do not have the same response towards changes in temperature (Boone et al. 1998; Lee et al. 2003). In this study, we therefore only consider heterotrophic respiration originating from a managed bare soil.

Many field studies used a classical regression method to determine the temperature sensitivity of soil respiration. This method does not account for the confounding factors discussed above. Another uncertainty of this method is related to the choice of measurement depth/volume to relate soil temperature and soil respiration. For example, the attenuation and phase shift of the soil temperature amplitude vary with soil depth (Bahn et al. 2008; Pavelka et al. 2007; Reichstein and Beer 2008), which means that different temperature responses will be found for different temperature measurement depths (e.g. Graf et al. 2008; Pavelka et al. 2007; Xu and Qi 2001).

Recently inverse modelling using process-based models has been increasingly used for a more reliable quantification of the response of soil respiration to environmental variables (e.g. Carvalhais et al. 2008; Scharnagl et al. 2010). For example, Weihermüller et al. (2009) presented a laboratory experiment to determine the soil water content response function of soil respiration using inverse modelling. An inverse modelling approach has also been used to determine global scale temperature and soil water content sensitivity of soil respiration by analysis of observed soil organic carbon contents with a mechanistic decomposition model (Ise and Moorcroft 2006). Zhou et al. (2009) inversely estimated the global spatial pattern of temperature sensitivity (Q_{10} values) from measured soil organic carbon content. A comprehensive overview of parameter estimation within the field of terrestrial carbon flux studies was provided by Wang et al. (2009). The performance of different parameter estimation methods was compared by Fox et al. (2009) and Trudinger et al. (2007).

The aim of this paper is to evaluate a new method to simultaneously estimate the response of soil respiration to changes in temperature and soil water content from field soil respiration measurements. The new method is based on inverse modelling using a detailed CO_2 production and transport model explicitly accounting for soil temperature and water content variations. The data set used for inverse modelling consisted of measurements of soil respiration, soil temperature, and soil water content at a high temporal resolution and for a comparably long period. The SOILCO2/RothC-model (Herbst et al. 2008) was used for the simulation of water flux, heat flux, CO_2 transport, and CO_2 production. To investigate whether the choice of functional relationship between temperature and soil respiration affected the inverse modelling results, we tested four common functional approaches in combination with a single soil water content response function.

Materials and methods

Model description

We used the 1-dimensional numerical model SOILCO2/RothC to predict soil water content, soil temperature, CO_2 production, and CO_2 transport. In the following we provide a brief model description. For detailed information, we refer to Šimůnek and Suarez (1993) and Herbst et al. (2008).

The water flow is described by the Richards equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} - 1\right)\right] - Q \qquad (1)$$

where θ is the volumetric water content (cm^3 cm^{-3}), t is time (h), z is the depth (cm), K is the unsaturated hydraulic conductivity (cm h^{-1}), h is the pressure head (cm), and Q is a source/sink term (cm^3 cm^{-3} h^{-1}). The soil water retention $\theta(h)$ and hydraulic conductivity $K(h)$ functions are described by the Mualem-van Genuchten approach (van Genuchten 1980):

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^m} \qquad (2a)$$

$$K(h) = K_s S_e^{0.5}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \qquad (2b)$$

$$\text{with } S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad m = 1 - 1/n \quad n > 1 \qquad (2c)$$

where θ_r and θ_s are the residual and saturated water content (cm^3 cm^{-3}), α is the inverse of the bubbling pressure (cm^{-1}), K_s is the saturated hydraulic conductivity (cm h^{-1}), and m and n are shape parameters (–).

The transport of heat is calculated according to Sophocleous (1979) by:

$$C\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda(\theta)\frac{\partial T}{\partial z}\right] - C_w\frac{\partial J_w T}{\partial z} \qquad (3)$$

where T is the soil temperature (°C), λ is the thermal conductivity of the soil (kg cm h^{-3} °C^{-1}), C and C_w are the volumetric heat capacities (kg h^{-2} cm^{-1} °C^{-1}) of the porous medium and the liquid phase, and J_w is the water flux density (cm h^{-1}). It should be noted that water and heat transport are coupled through the dependence of the thermal conductivity on water content and the convective transport of heat with the water flux J_w.

After the solution of the water and heat transport equations, the transport equation for carbon dioxide is solved considering the CO_2 flux caused by diffusion in the gas phase (J_{da}) (cm h^{-1}), the CO_2 flux caused by dispersion in the dissolved phase (J_{dw}) (cm h^{-1}), the CO_2 flux caused by convection in the gas phase (J_{ca}) (cm h^{-1}), and the CO_2 flux caused by convection in the dissolved phase (J_{cw}) (cm h^{-1}):

$$\frac{\partial c_T}{\partial t} = -\frac{\partial}{\partial z}(J_{da} + J_{dw} + J_{ca} + J_{cw}) - Qc_w + S \qquad (4)$$

where c_T is the total volumetric concentration of CO_2 (cm^3 cm^{-3}), S is the CO_2 production/sink term (cm^3 cm^{-3} h^{-1}), c_w is the CO_2 concentration in the liquid phase (cm^3 cm^{-3}), and Q is the root water uptake (cm^3 cm^{-3} h^{-1}).

Soil organic matter decomposition (i.e. heterotrophic respiration) is described by the RothC pool concept as sketched in Fig. 1 (Coleman and Jenkinson 2005; Jenkinson 1990). In this concept, fresh plant input entering the soil consists of decomposable plant material (DPM) and resistant plant material (RPM). The proportion of DPM and RPM depends on the plant material, i.e. for agricultural crops and improved grassland the DPM/RPM ratio is 1.44 according to Jenkinson (1990). Both pools undergo decomposition, and part of the decomposed carbon fraction is released from the soil as CO_2. The remaining fraction of decomposed carbon is used to form microbial biomass (BIO) and humified organic matter (HUM). Both the BIO and HUM pool are decomposed to form further BIO, HUM, and CO_2. The proportion of CO_2/(BIO + HUM) is a function of the clay content of the soil. Besides these four active pools, one part of SOM is considered to be inert (IOM). Decomposition of the active carbon pools is described by first order kinetics:

$$\frac{\partial C_{p,i}}{\partial t} = -\lambda_{p,i,0} f_T f_W C_{p,i} \qquad (5)$$

where $C_{p,i}$ is the ith pool concentration (kg C cm^{-3}), and $\lambda_{p,i,0}$ is the decomposition constant of the ith pool, which are 10, 0.3, 0.66, and 0.02 year^{-1} for the DPM, RPM, BIO, and HUM pool, respectively. The decomposition constants are valid for optimal conditions of soil water, aeration, and a reference temperature. f_T and f_W are response functions (–) for soil temperature and soil water content, respectively.

Soil water content and temperature response functions

The availability of water is essential for soil microbial activity. Increasing soil water content enhances

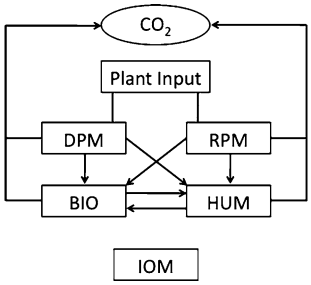

Fig. 1 Schematic overview of the RothC pool concept (modified from Jenkinson 1990). Carbon is exchanged between four active pools: decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO), and humified organic matter (HUM). The fifth pool is inert organic matter (IOM)

substrate diffusion. However, the supply of oxygen is reduced when the soil water content is high (Skopp et al. 1990). As a consequence, increasing water content first enhances microbial activity, but becomes repressive for water contents higher than some optimum. We used the following relationship to describe the soil water content response f_W:

$$f_w(\theta) = \frac{\exp\left(a_W\theta + b_W\theta^2\right)}{\exp\left(\frac{-a_W^2}{4b_W}\right)} \tag{6}$$

where a_W and b_W are empirical parameters. The denominator is a normalisation factor used to obtain a maximum value of 1 at the optimal water content, θ_{opt}, which is located at:

$$\theta_{opt} = -\frac{a_W}{2b_W} \tag{7}$$

For the temperature response, we used several common approaches from literature. First, we used the temperature reduction function of the RothC pool concept in its original parameterisation:

$$f_{T,orig} = \frac{47.9}{1 + \exp\left(\frac{106}{T+18.3}\right)} \tag{8}$$

$f_{T,orig}$ is equal to 1 at a reference temperature T_{ref} of 9.25°C. This formulation can be rescaled to another reference temperature by the following approach:

$$f_T = \frac{f_{T,orig}}{f_{Tref,orig}} \tag{9}$$

Second, we used a modified form of the Arrhenius relationship (e.g. Fang and Moncrieff 1999; Šimůnek and Suarez 1993):

$$f_T = \exp\left(\frac{E(T - T_{ref})}{R(273.15 + T)\,(273.15 + T_{ref})}\right) \tag{10}$$

where E is the activation energy of the reaction (kg m^2 s^{-2} mol^{-1}) and R is the universal gas constant (8.314 kg m^2 s^{-2} K^{-1} mol^{-1}). Both the RothC and the Arrhenius approach can only describe an increase in microbial decomposition with increasing temperature. Additionally, we analysed relationships with an optimal temperature and a potential decrease of microbial decomposition for high temperature. The first relationship of this type is an exponential equation according to O'Connell (1990):

$$f_T = \exp\left(a_1 + b_1 T\left(1 - 0.5T/T_{opt}\right)\right) \tag{11}$$

where a_1 and b_1 are empirical parameters and T_{opt} is the optimum temperature. The second relationship of this type was introduced by Parton et al. (1987):

$$f_T = a_2 + b_2 T^{d_2} - (T/c_2)^{e_2} \tag{12}$$

where a_2, b_2, c_2, d_2, and e_2 are empirical parameters. Negative values for these temperature response functions were set to 0.

Determination of the activation energy from linear regression analysis

Conventionally, the activation energy of soil respiration is derived from a linear regression analysis based on the Arrhenius formulation (Johnson and Thornley 1985) according to:

$$\lambda = \beta \exp\left(\frac{-E}{R(T + 273.15)}\right) \tag{13}$$

where β (h^{-1}) is a constant. This formulation can be linearised using a log-transform:

$$\log_e \lambda = \log_e \beta - \frac{E}{R(T + 273.15)} \tag{14}$$

The activation energy can then be calculated from the slope p_1 according to:

$$E = -p_1 R \tag{15}$$

Field measurements

All measurements were made at the FLOWatch test site, which is located in the river Rur catchment

(North Rhine-Westphalia, Germany). The soil was classified as a Cutanic Luvisol (Ruptic, Siltic) according to World Reference Base for Soil Resources classification (IUSS Working Group WRB, 2007) and consists of three horizons ranging from 0 to 33 cm (Ap), 33 to 57 cm (EBw), and 57 to 130+ cm (2Btw). The soil texture is a silt loam. A detailed description of the test site is given by Weihermüller et al. (2007). Our investigation covered the time period from October 2006 until October 2007. CO_2 flux measurements were only available until September 2007. During this period, weeds were continuously removed manually and/or by herbicide (glyphosate) application.

Soil temperature was measured at 0.5, 3, 5, and 10 cm depth by type T thermocouples and at 15, 30, 45, 60, 90, and 120 cm depth by pF-meters (Ecotech, Bonn, Germany). Soil water content was measured at 15, 30, 45, 60, 90, and 120 cm depth from April to October 2007 by custom made 3 rod TDR probes with a rod length of 20 cm. All TDR probes were connected to a Campbell multiplexing and data logging system (Campbell Scientific, Logan, UT, USA). The raw waveforms were stored and analysed semi-automatically using the Matlab routine TDR-Ana developed in the Forschungszentrum Jülich GmbH, which follows the principles suggested by Heimovaara and Bouten (1990). Matric potentials were recorded at 120 cm by pF-meters (Ecotech, Bonn, Germany). Climatic data were obtained from the meteorological tower of the Research Centre Jülich GmbH (5.4 km NW from the test site).

CO_2 fluxes were measured by automated soil CO_2 flux chambers (Li-8100, Li-Cor Inc., Lincoln, NE, USA) operated with the Li8100 multiplexer system. From October 2006 to April 2007, CO_2 fluxes were measured twice an hour using a single chamber. In April 2007, we installed a three chamber multiplexer system that measured 4 times per hour. All chambers were placed on a soil collar with a diameter of 20 cm and a height of 7 cm, of which 5 cm were belowground. Each chamber was closed for 2 minutes and the rise in CO_2 concentration was measured with an infrared gas analyser. To estimate the CO_2 flux, a linear regression was fitted to the measured CO_2 concentrations. Finally, hourly mean CO_2 fluxes and standard deviations were calculated. In order to remove outliers, we did not consider fluxes with a standard deviation larger than 5 times the mean standard deviation.

In April 2007, the soil collars were temporarily removed and the entire field was power-harrowed. Because a large amount of weed was present at the field site surrounding the flux measurement plot, this harrowing caused a significant biomass input at the location of the collars, which were re-installed after harrowing. During summer 2007, a sporadic occurrence of seedlings was observed at the plot. The removing of the weeds by hand ensured a minimal contribution of autotrophic respiration to the measured CO_2 flux.

To characterise the organic carbon within the Ap-horizon, disturbed samples were taken from three depths (0–10, 10–20, and 20–30 cm) in October 2006. Additionally, mixed soil samples from three locations were taken from deeper depths (30–40, 40–50, 50–60, 60–100 cm) in June 2007. The organic carbon content of the soil samples was analysed using a Leco CHNS-932 analyser (St. Joseph, MI, USA).

Model parameterisation and initialisation

Since measured data were not available at the beginning of the simulation, the initial soil water content profile was derived from measurements for a comparable period in 2007. An atmospheric boundary condition was used to describe the upper boundary. The reference potential evapotranspiration was estimated according to the FAO guidelines (Allen et al. 1998) from measured atmospheric temperature, precipitation, wind speed, atmospheric pressure, relative humidity, and actual duration of sunshine. The potential evaporation of a bare soil was calculated from the reference potential evapotranspiration by multiplication with a factor of 1.15 (Allen et al. 1998). The lower boundary was described by measured matric potentials. Figure 2 shows the precipitation and potential evaporation for the study period. The total precipitation was 831 mm and the total potential evaporation was 757 mm.

The initial conditions and the upper and lower boundary conditions for heat transport were derived from measured soil temperatures. Missing surface temperatures (T_{surf}) were estimated from atmospheric temperatures (T_{atm}) using a linear regression function ($T_{surf} = 1.1173T_{atm} - 0.9057;\ R^2 = 0.88$). Missing temperatures in 120 cm soil depth were estimated by linear interpolation. The parameters for the thermal

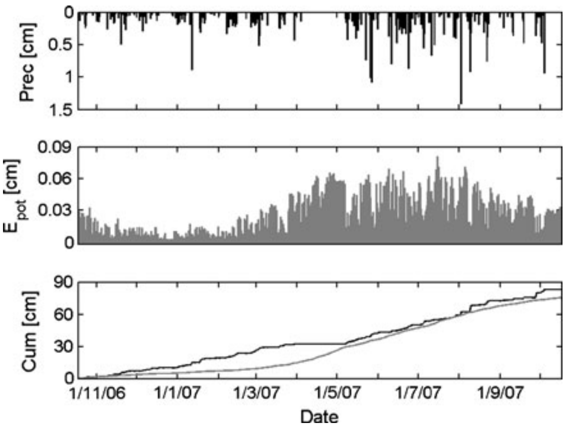

Fig. 2 Precipitation (Prec), potential evaporation (E_{pot}), cumulative precipitation (*black*) and potential evaporation (*grey*) between October 2006 and October 2007

conductivity of a loamy soil were taken from Chung and Horton (1987), and are summarised in Table 1.

Initial CO_2 concentrations within the soil profile were taken from a forward model run from a comparable period in 2007. CO_2 concentration at the soil surface was set to the atmospheric concentration of 0.038%. The lower boundary was defined as a zero flux boundary. All additional CO_2 transport parameters are summarised in Table 1.

The initial carbon pool sizes were determined from measured soil carbon fractions. Therefore, a physical fractionation procedure was used, which is based on wet sieving after chemical dispersion and was proposed by Cambardella and Elliott (1992) and Skjemstad et al. (2004). An amount of 10 g soil (<2 mm) was shaken overnight with 0.05 l of fresh Na-hexametaphosphate solution (5 g l^{-1}). Afterwards, the dispersed soil was sieved sequentially using a 200 μm (Retsch GmbH, Haan, Germany) and a 53 μm sieve (Fritsch GmbH, Idar-Oberstein, Germany) and rinsed thoroughly with water until the rinsate was clear. The remaining material (200–2000 μm, 53–200 μm) was freeze-dried and weighed. The 0–53 μm soil fraction contains the mineral-associated and water-soluble carbon, while the 53–2000 μm soil fraction contains the particulate organic matter (POM). According to Skjemstad et al. (2004) the RPM fraction C_{RPM} of the SOILCO2/RothC model was set to the measured POM fraction (53–2000 μm). The size of the IOM pool was set to the MIR-measured black carbon fraction (Bornemann et al. 2008). We assumed that the DPM fraction at the beginning of the simulation was negligible. The fraction of HUM and BIO was calculated as the remaining fraction (RF) from the total organic carbon [$RF = C_{HUM} + C_{BIO} = C_{org} - (C_{DPM} + C_{RPM} + C_{IOM})$]. The proportion between BIO and HUM was assumed to be 0.0272 according to Zimmermann et al. (2007). Since no information about SOM composition for soil layers deeper than 30 cm was available at the beginning of the simulation period, we used the SOM composition determined 8 months later and assumed that SOM was not significantly altered in the deeper soil horizons. This assumption was later confirmed by our simulations, which indicate that the mean carbon loss from the RPM pool was only 4% in the 30–60 cm depth range for the entire study period. Carbon pool concentrations were linearly interpolated between the measurement depths.

In Table 2 the measured concentration of SOM, POM (=RPM), and black carbon (=IOM) are summarised. Furthermore, the calculated remaining fraction (RF = HUM + BIO) and percentages of the several fractions are given. As expected, total SOM contents decreased with depth. Both, concentration and percentage of the fast decomposing RPM pool and the slow decomposing HUM pool decreased with depth. Contrarily, the proportion of the inert IOM pool significantly increased with depth. The observed soil carbon distribution characterised by decreasing concentrations and increasing recalcitrance in combination with decreasing soil temperatures in the soil profile cause a strong decrease of CO_2 production with soil depth, as is typically observed in field studies (e.g. Köhler et al. 2010; Suarez and Simunek 1993).

Fresh weed material entered the upper 15 cm of the soil after soil harrowing in April 2007. For different crop stands, crop rotations, and fertilization rates various authors proposed annual carbon inputs via roots and crop residuals ranging from 1.5 to more than 3.8 t C ha^{-1} (Coleman and Jenkinson 1996; Coleman et al. 1997; Falloon et al. 1998; Jenkinson and Coleman 1994). In many of these cases, large proportions of the plant material were removed by harvesting. Due to the way the test site was managed during this experiment (no removal of aboveground weed biomass), rather large amounts of fresh plant material were incorporated into the soil during harrowing. Therefore, we assumed a total input of 3 t C ha^{-1}.

Table 1 Heat (Chung and Horton 1987) and CO_2 transport parameters (Patwardhan et al. 1988) used in the numerical simulation

Parameter	Value	Unit
Heat transport		
Thermal dispersivity	1.5	cm
Empirical constant b_1 of soil thermal conductivity function	1.134E+12	kg cm^{-1} h^{-3} °C^{-1}
Empirical constant b_2 of soil thermal conductivity function	1.834E+12	kg cm^{-1} h^{-3} °C^{-1}
Empirical constant b_3 of soil thermal conductivity function	7.157E+12	kg cm^{-1} h^{-3} °C^{-1}
CO_2 transport		
Molecular diffusion coefficient of CO_2 in air at 20°C	572.4	cm^2 h^{-1}
Molecular diffusion coefficient of CO_2 in water at 20°C	0.0637	cm^2 h^{-1}
Longitudinal dispersivity of CO_2 in water	1.5	cm

Table 2 Measured carbon concentration of total soil organic matter (SOM), particulate organic matter (POM), and black carbon (BC) in the soil profile

Depth (cm)	SOM (mg C cm^{-3})	POM (mg C cm^{-3})	BC (mg C cm^{-3})	RF (mg C cm^{-3})
0–10	18.54	3.30 (17.8%)	2.12 (11.4%)	13.12 (70.8%)
10–20	17.87	2.50 (14.0%)	2.43 (13.6%)	12.94 (72.4%)
20–30	17.21	2.50 (14.5%)	2.52 (14.6%)	12.19 (70.8%)
30–40	7.92	0.51 (6.4%)	1.93 (24.4%)	5.48 (69.2%)
40–50	5.62	0.29 (5.2%)	1.71 (30.4%)	3.62 (64.4%)
50–60	4.72	0.23 (4.9%)	1.42 (30.1%)	3.07 (65.0%)
60–100	4.26	0.21 (4.9%)	1.35 (31.7%)	2.70 (63.4%)

RF is the remaining fraction (RF = SOM – POM − BC)

In brackets the percentages of POM, BC and RF from SOM are given

Inverse parameter estimation

To find the set of model parameters that best describe the measurements, the global optimisation algorithm SCE-UA (shuffled complex evolution method developed at the University of Arizona) was used (Duan et al. 1992, 1994). Optimisation methods are tools to find the minimum of a cost function that expresses the distance between simulated and measured data. Global search methods are more successful in finding the global minimum of a cost function compared to gradient-based methods which can get trapped in local minima (Wang et al. 2009). The SCE-UA algorithm searches the global optimum parameter combination within a feasible parameter space defined by the user using a set of complexes which initially are populated with points randomly distributed in the feasible parameter space. Each complex is made to evolve in the direction of improvement (minimum of the cost function) using the local-search simplex method (Nelder and Mead 1965). At periodic stages in the evolution, the entire population of points is shuffled and points are reassigned to complexes based on their performance to ensure information sharing. A detailed description of the SCE-UA algorithm is provided by Duan et al. (1994). The SCE-UA algorithm has been shown to be a powerful tool for calibration of hydrological models (Madsen et al. 2002) and has been successfully applied in other application areas (e.g. Bauer et al. 2008; Peters and Durner 2008). In this study, the cost function was defined by the sum of squared residuals (SSR):

$$\mathrm{SSR} = \sum_{i=1}^{k} \left(y_{\mathrm{obs},i} - y_{\mathrm{sim},i}\right)^2 \qquad (16)$$

where y_{obs} and y_{sim} are the observed and simulated data, respectively, and k is the number of data pairs available to compare observation and simulation.

For a reliable prediction of the water transport, the hydraulic parameters of four soil layers were inversely estimated. To reduce the number of estimated parameters, we assumed that the saturated and residual water contents were constant over the entire soil profile. This assumption is in good agreement with laboratory results for the same location, where the mean saturated water content is 0.39 $cm^3\ cm^{-3}$ with a standard deviation of only 0.03 $cm^3\ cm^{-3}$. In total, we estimated 14 hydraulic parameters (one θ_s and θ_r for the entire profile and α, n, and K_s for each layer). Additionally, we imposed a decrease of K_s with depth. We used 3899 water content measurements at 15, 30, 45, 60, and 90 cm, respectively and 2247 measurements at 120 cm depth in the inversion. In a second step, we inversely estimated the parameters of the soil water content response equation (Eq. 6) and the temperature response equations (Eqs. 8–12) from 6269 CO_2 flux measurements. For both optimization runs, SCE-UA was stopped when the change of the objective function was less than 0.1% in 10 consecutive loops, as recommended by previous studies with this optimization algorithm (Mertens et al. 2005).

Statistical criteria of model quality

Three criteria were used to judge the quality of the model simulations. First, we calculated the coefficient of determination R^2 (Ahrens 2003):

$$R^2 = \left(\frac{\sum_{i=1}^{k} \left(y_{\mathrm{obs},i} - \overline{y_{\mathrm{obs}}}\right)\left(y_{\mathrm{sim},i} - \overline{y_{\mathrm{sim}}}\right)}{\sqrt{\sum_{i=1}^{k} \left(y_{\mathrm{obs},i} - \overline{y_{\mathrm{obs}}}\right)^2 \sum_{i=1}^{k} \left(y_{\mathrm{sim},i} - \overline{y_{\mathrm{sim}}}\right)^2}} \right)^2 \tag{17}$$

where $\overline{y_{\mathrm{obs}}}$ and $\overline{y_{\mathrm{sim}}}$ are the arithmetic means of the observed and simulated data, respectively. The model efficiency ME (Nash and Sutcliffe 1970) was used as a second criterion:

$$\mathrm{ME} = 1 - \frac{\sum_{i=1}^{k} \left(y_{\mathrm{obs},i} - y_{\mathrm{sim},i}\right)^2}{\sum_{i=1}^{k} \left(y_{\mathrm{obs},i} - \overline{y_{\mathrm{obs}}}\right)^2} \tag{18}$$

A model efficiency close to 1 indicates that observed and simulated data are closely related and without systematic bias. In contrast, a model efficiency lower than 0 means that the mean is a better predictor of the data than the applied model. In order to identify the best model taking into account both goodness of fit and model complexity, Akaike's information criterion (AIC, Akaike 1974) was used:

$$\mathrm{AIC} = -2 \log_e L_{\max} + 2m \tag{19}$$

where $\log_e L_{\max}$ is the maximum log-likelihood function and m is the number of model parameters. Assuming normally distributed errors, AIC can be written as:

$$\mathrm{AIC} = n \log_e \left(\frac{\sum_{i=1}^{n} \left(y_{\mathrm{obs},i} - y_{\mathrm{sim},i}\right)^2}{n} \right) + 2(m+1) \tag{20}$$

The lowest AIC value identifies the best model.

Results and discussion

Simulation of soil water content and soil temperature

The measured soil water content could not be sufficiently described by the model with one set of hydraulic parameters for the plough horizon Ap (upper 33 cm). Corresponding to the findings of Abbaspour et al. (2000), the Ap horizon had to be divided into two separate layers with different hydraulic properties to obtain an adequate reproduction of the measured soil water content (Fig. 3). The Ap horizon was divided at a depth of 20 cm, which is the maximum penetration depth of the power harrow. The hydraulic properties yielding the best prediction of measured soil water content are summarised in Table 3. The resulting high n value ($n = 1.97$) of the upper soil layer is not representative for a silt loam soil, which might be due to the large coarse fraction (10–15 mass% >2 mm). In addition, the soil structure of this upper layer was changed due to tillage. However, the water flow of the upper soil layer was predicted well and 87% of the variation in soil water content measured at 15 cm depth was explained (Fig. 3). At 90 and 120 cm depth, model efficiency was negative indicating that the mean soil water content at these depths is a better predictor than the model, which is largely the result of the low dynamics in water content (Fig. 3). However, simulated water content was within the uncertainty range of measured values. Furthermore, slight deviations in soil water content of the lower soil layers do not have any significant influence on the estimation of temperature and soil water content response parameters

Fig. 3 Measured (*grey symbols*) and simulated (*black lines*) water contents at different soil depths

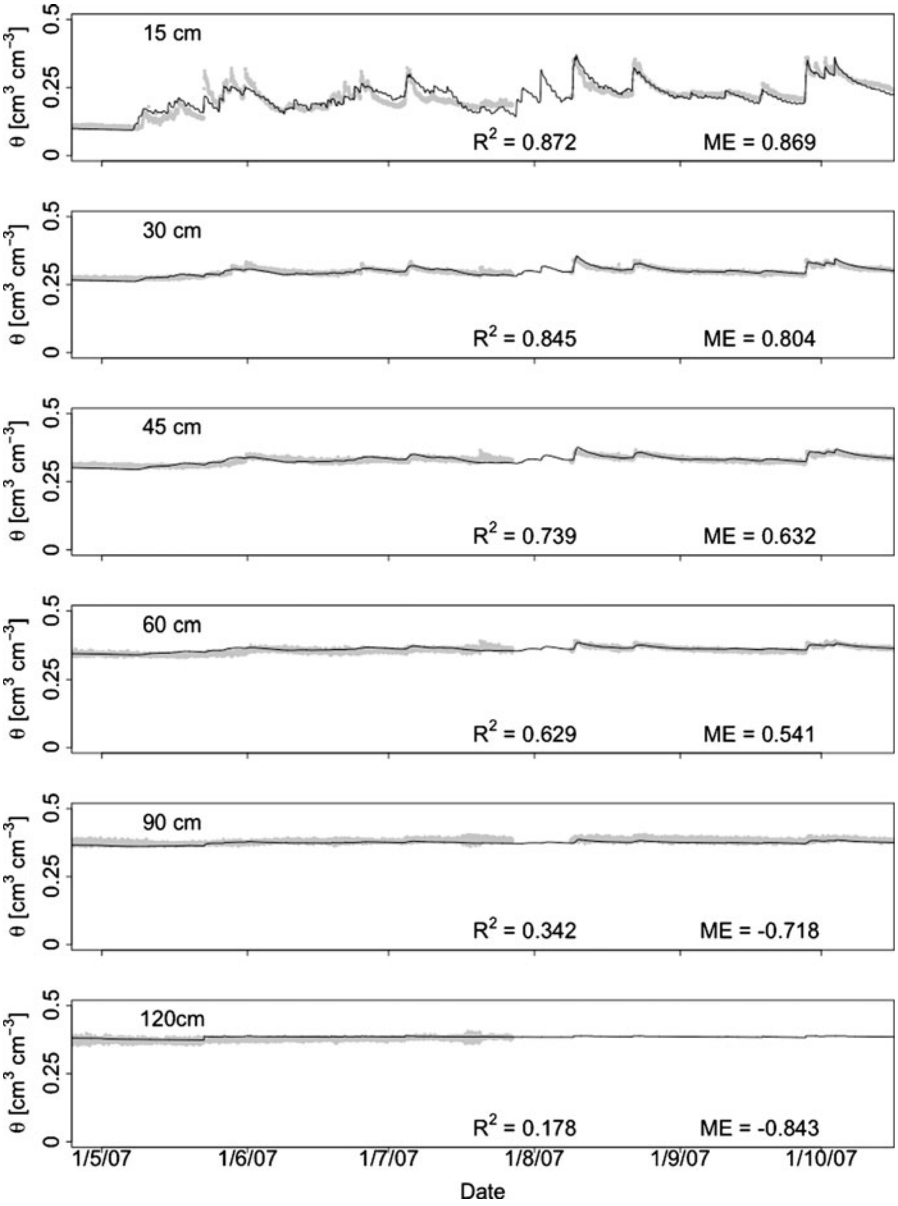

Table 3 Estimated hydraulic parameters according to the Mualem-van Genuchten approach (van Genuchten 1980) of the soil layers

Layer	Depth (cm)	θ_r (cm^3 cm^{-3})	θ_s (cm^3 cm^{-3})	α (cm^{-1})	n (–)	K_s (cm h^{-1})
1	0–20	0.008	0.389	0.012	1.97	3.82
2	20–33	0.008	0.389	0.023	1.23	2.64
3	33–57	0.008	0.389	0.011	1.30	2.12
4	57–120	0.008	0.389	0.007	1.22	0.28

Note that θ_r and θ_s were assumed to be constant with depth to reduce number of parameters for the estimation

θ_r residual water content, θ_s saturated water content, α inverse of the bubbling pressure, n parameter, K_s saturated hydraulic conductivity since released CO_2 mainly originates from soil organic matter decomposition within the upper soil horizons.

Measured soil temperature was generally predicted well by the model (Fig. 4). However, soil temperature was overestimated by up to 3°C for the first soil layers from mid-November to early January. This is a result of the fact that only few surface temperature measurements were available during this period, and therefore, surface temperatures were estimated from atmospheric temperatures.

Simulation of CO_2 fluxes

To determine the temperature and soil water content response, which are most appropriate to describe the measured CO_2 fluxes, the parameters of all possible combinations of the soil water content response function (Eq. 6) and the five different temperature response functions (Eqs. 8–12) were inversely estimated by minimizing the difference between measured and modelled CO_2 fluxes. For the different combinations of response functions between 2 and 7 parameters were estimated. The results are summarised in Table 4. Data and model were not in agreement when the original parameterisation of the RothC temperature response equation was used. Prediction of measured CO_2 fluxes was significantly improved when the RothC temperature response equation was scaled to another optimised reference temperature (Sum of Squared Residuals, SSR, decreased from 812 to 632 $(\text{kg C ha}^{-1}\ \text{h}^{-1})^2$). The data were best described by the approach of Parton et al. (1987) with a SSR value of 538 $(\text{kg C ha}^{-1}\ \text{h}^{-1})^2$. However, the Arrhenius and O'Connell (1990) equations produced just slightly larger errors (SSR of 542 and 547 $(\text{kg C ha}^{-1}\ \text{h}^{-1})^2$, respectively). The Parton temperature response function resulted in the smallest value of Akaike's information criterion, which suggests that this response function provides the best balance between goodness of fit and model complexity. We therefore use this equation to analyze the difference between measured and predicted soil respiration.

In Fig. 5, the measured and simulated CO_2 flux is shown for the temperature response equation according to Parton et al. (1987). Furthermore, the distribution of CO_2 released during decomposition, soil water content, and soil temperature in the upper soil horizon (0–33 cm) are illustrated. Contrary to the continuous distribution of soil temperature, a distinct boundary is visible in 20 cm depth for soil water content due to the different hydraulic properties of the soil layers (Table 3). This boundary is also visible in the CO_2 distribution since soil organic matter decomposition also depends on the soil water content. The modelled vertical distributions of CO_2 concentrations are quite similar to the concentration distributions measured for bare soils under comparable conditions (Suarez and Simunek 1993; Yasuda et al. 2008).

In general, the course of measured CO_2 fluxes was well described by the model. In January 2007, soil surface temperatures dropped below 0°C resulting in a depression of CO_2 production. This freezing period was followed by a strong CO_2 release up to 1.4 kg C $\text{ha}^{-1}\ \text{h}^{-1}$. A possible explanation for the observed CO_2 flush is the death of microbial biomass due to the low temperature and the subsequent decomposition of this new carbon source with increasing soil temperatures and reactivated microbial activity (e.g. Matzner and Borken 2008). Since the model can currently not describe this process, the measurements of this period were not considered to avoid bias in the inverse parameter estimation procedure. The simulations indicate that 90% of CO_2 was produced within the upper soil horizon (0–33 cm) where CO_2 production was notably high in the upper 15 cm of the soil profile in May and June 2007. In the last half of April and the first half of May 2007, the soil surface layer was almost dry. The low water content obviously hampered SOM decomposition since CO_2 fluxes were significantly lower than in the following period despite high temperatures and fresh carbon input in April 2007 due to the harrowing.

High measured CO_2 fluxes were systematically underestimated during the first half of June 2007. The higher uncertainty in the measured CO_2 fluxes during this period expressed by the high standard deviations of up to 1.5 kg C ha^{-1} cannot completely explain the observed mismatch. Probably, additional CO_2 was released by decomposed plant roots, which remained in the soil after the manual weed removal (Herbst et al. 2008). The period of highest soil temperatures in July 2007 was not accompanied by highest CO_2 fluxes despite moderate soil water contents. This can be explained by the decrease of the fresh litter input quantity and quality during the course of

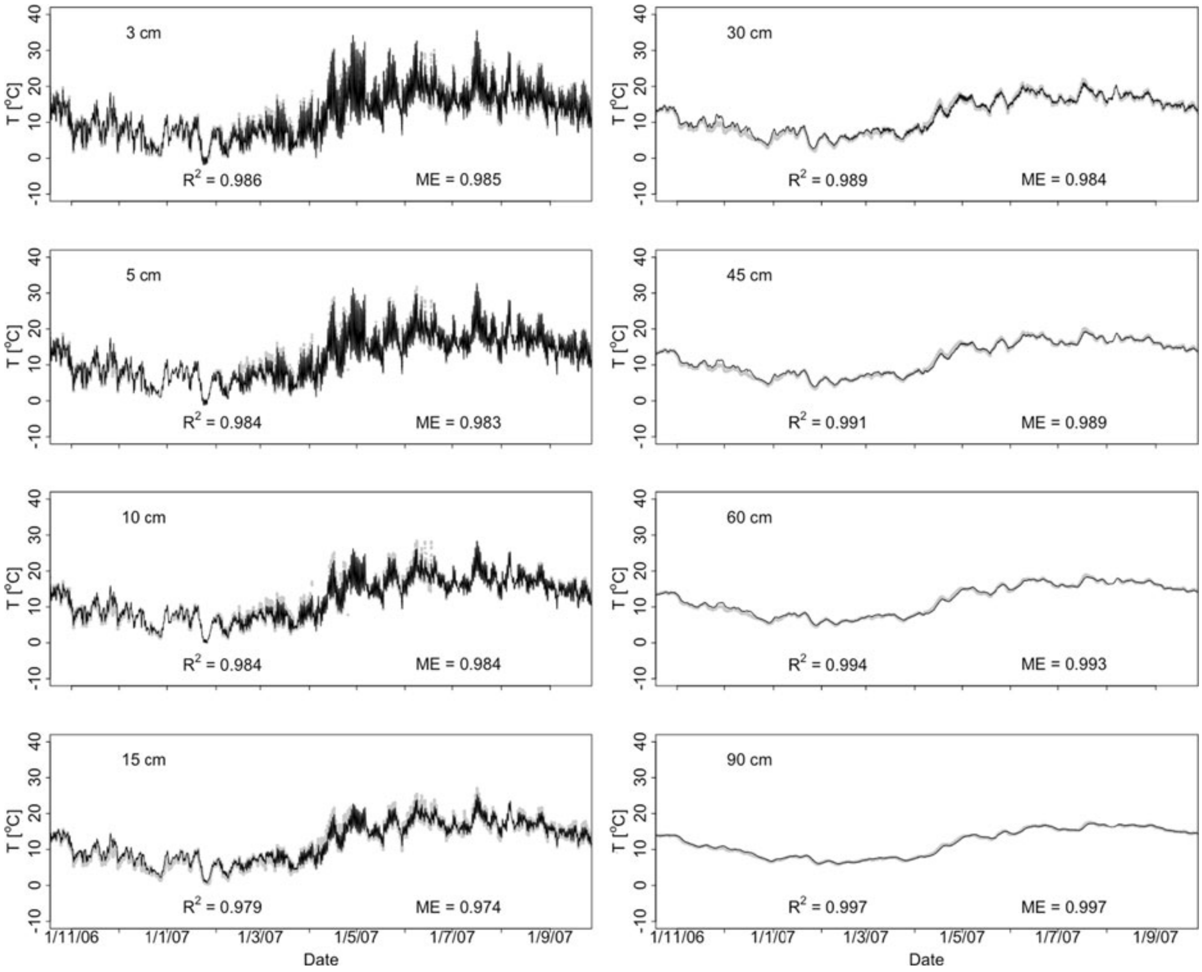

Fig. 4 Measured (*grey*) and simulated (*black*) temperature in different soil depths

decomposition, which is supported by the findings of Leifeld and Fuhrer (2005) and Larionova et al. (2007).

Figure 6 presents the four temperature response functions obtained using inverse modelling. The RothC function clearly deviates from the other three functions. This can be explained by the limited flexibility of the RothC function where only the reference temperature was variable and the curvature was fixed. The other three functions are very similar for temperatures below 25°C. As stated before, the Parton response function is the best approach in regard to both, goodness of data prediction and complexity (number of model parameters) (Table 4). For temperatures above 25°C, the three functions highly diverge. The reasons for the uncertainty in the course of the temperature response function for high temperatures are twofold. Temperatures above 25°C only occurred up to a maximum depth of 18 cm, and temperature exceeded 25°C only 1.6% of the time. It is important to stress here that the scaled temperature functions can be only used in the range of soil temperature used for calibration and to a point where the functions match each other (maximum temperature of 25°C). For higher soil temperatures that might occur due to climate change, these temperature functions have to be treated carefully.

The optimized soil water content responses are also shown in Fig. 6. The curvatures of the soil water content response equations combined with the temperature response function of Arrhenius, O'Connell (1990), and Parton et al. (1987) are very similar. The calculated optimal water content was 0.24 cm^3 cm^{-3}, which corresponds to a water filled pore space of

Table 4 Prediction of measured CO_2 fluxes using different approaches for the temperature response

Temperature response	Estimated temperature parameters	Estimated soil water content parameters	SSR [(kgC $ha^{-1})^2$]	R^2 (–)	ME (–)	AIC (–)	$\overline{y_{sim}}$ (kg C ha^{-1})
$RothC_{orig}$ (Eq. 8)	–	$a_W = 157.81$ $b_W = -360.44$	812	0.626	0.596	−12,806	0.457
$RothC_{scale}$ (Eqs. 8, 9)	$T_{ref} = 14.3°C$	$a_W = 58.16$ $b_W = -126.30$	632	0.697	0.685	−14,378	0.421
Arrhenius (Eq. 10)	$T_{ref} = 15.5°C$ $E = 98$ kJ mol^{-1}	$a_W = 64.91$ $b_W = -136.39$	547	0.729	0.727	−15,282	0.409
O'Connell (Eq. 11)	$a_1 = -3.3416$ $b_1 = 0.2611$ $T_{opt} = 42.64$	$a_W = 60.90$ $b_W = -127.55$	542	0.730	0.730	−15,340	0.399
Parton (Eq. 12)	$a_2 = 0.2073$ $b_2 = 0.0001$ $c_2 = 31.52$ $d_2 = 3.254$ $e_2 = 75.69$	$a_W = 61.44$ $b_W = -128.50$	538	0.733	0.732	−15,374	0.405

SSR sum of squared residuals, R^2 coefficient of determination, *ME* model efficiency, $\overline{y_{sim}}$ arithmetic mean of simulated respiration

62%. This value is in good agreement with many other studies that found optimal aerobic microbial activity between 50 and 80% water filled pore space (e.g. Greaves and Carter 1920; Pal and Broadbent 1975; Rixon and Bridge 1968; Rovira 1953; Seifert 1961; Weihermüller et al. 2009). Overall, the good agreement between the temperature and soil water content response equations despite different functional forms indicates that the inverse modelling approach is a useful tool to obtain reliable estimates of the temperature and soil water content response.

Measured soil respiration was reasonably described by our optimised model setup. However, there are still differences between simulated and measured soil respiration (Table 4). The mismatch between measured and modelled soil respiration is on the one hand caused by measurement errors, on the other hand it is affected by model errors such as missing processes and errors in boundary conditions. Hence, a comprehensive uncertainty analysis is an important future step towards a more complete model-data integration approach (e.g. Wang et al. 2009; Williams et al. 2009).

Finally, it has to be noted that the inverse modelling analysis presented here leads to an independent estimate of the temperature and water content response function only because water content and temperature are not strongly correlated at our field site (maximum R^2 of 0.13 at the soil surface). Additionally, the response functions obtained by inverse modelling should be treated carefully if they are transferred to other process-based turnover models because any kind of model error is propagated into the estimation of the parameters of the response functions. Both the influence of covariance of the driving variables (soil water content and soil temperature) as well as the predictive uncertainty introduced by model errors should be evaluated in future synthetic model studies.

Comparison to conventionally determined temperature responses

Typically, the temperature response of soil respiration in field studies is quantified by fitting a regression between log-transformed CO_2 fluxes and temperatures measured in a certain soil depth (see "Determination of the activation energy from linear regression analysis" section). This practice has been criticised because confounding factors such as correlations with water (Davidson et al. 1998), or the effect of temperature measurement depth (Graf et al. 2008) might strongly affect the temperature sensitivity thus obtained. It is therefore insightful to compare the temperature sensitivity determined using inverse modelling, which simultaneously attempts to consider temperature, water content, and substrate availability effects, to

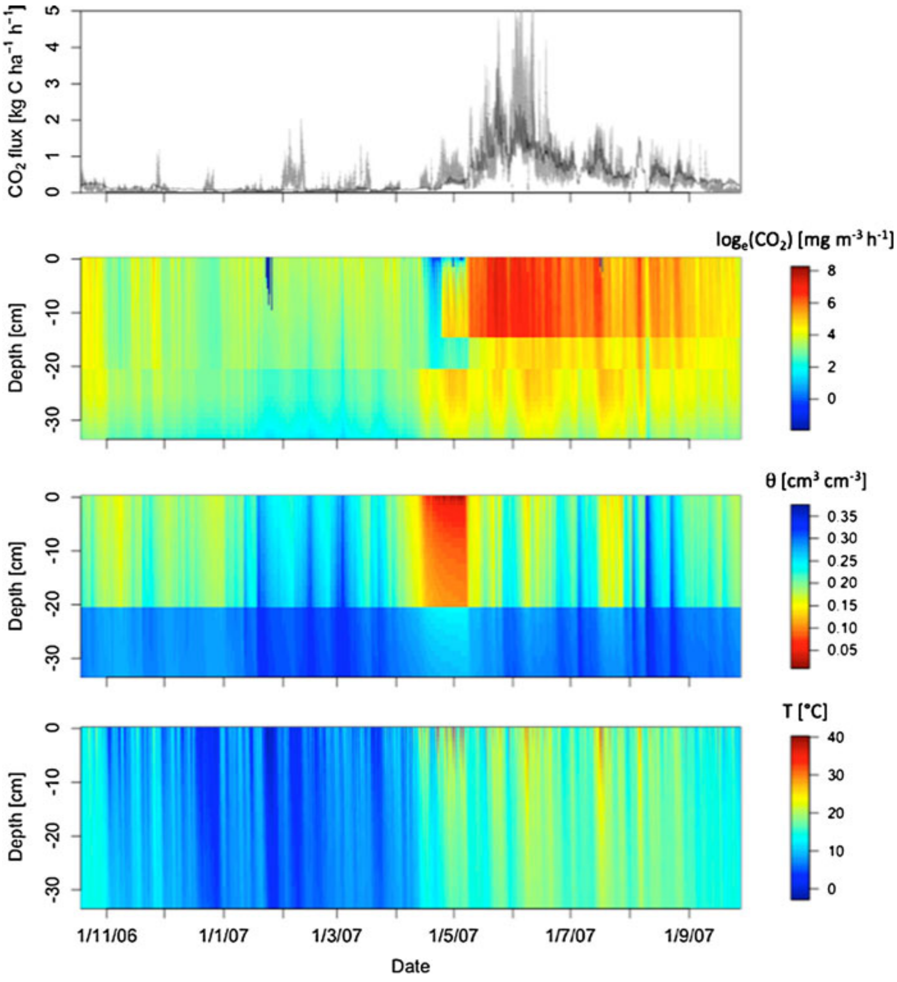

Fig. 5 Measured and modelled CO$_2$ flux using the soil water content response equation and the temperature response equation according to Parton et al. (1987). Measured CO$_2$ fluxes are shown as mean values with standard deviation (*grey*). Simulated CO$_2$ fluxes are illustrated as black line. Simulated CO$_2$ production, water content, and temperature are plotted for the plough horizon (upper 33 cm)

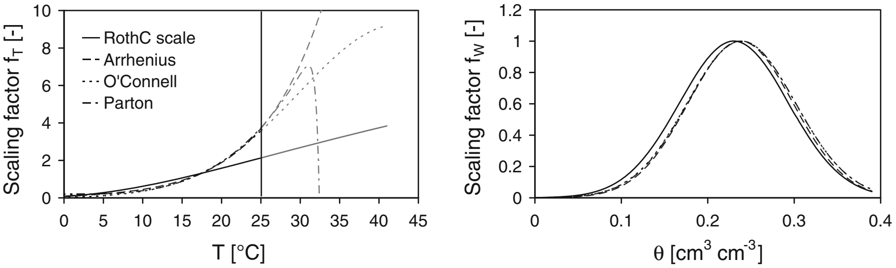

Fig. 6 Optimized temperature and soil water content response functions. Parameters for all functions are listed in Table 4

the one that would have been obtained using a linear regression that neglects confounding factors. For reasons of comparability between the two different methods of data analysis, we used simulated instead of measured soil temperatures in the linear regression. This is justified by the excellent model predictions for soil temperature (Fig. 4). As shown before, temperature response derived from the traditional regression analysis highly depends on the depth of the temperature measurement with apparently stronger temperature responses with increasing depth (Bahn et al. 2008; Graf et al. 2008; Pavelka et al. 2007). For temperature measurements at the soil surface, the linear regression analysis provided an activation energy of 92 kJ mol^{-1} and for temperature measurement at 10 cm depth, a much higher value of 126 kJ mol^{-1} was obtained (Fig. 7). This clearly illustrates the ambiguity of the classical regression

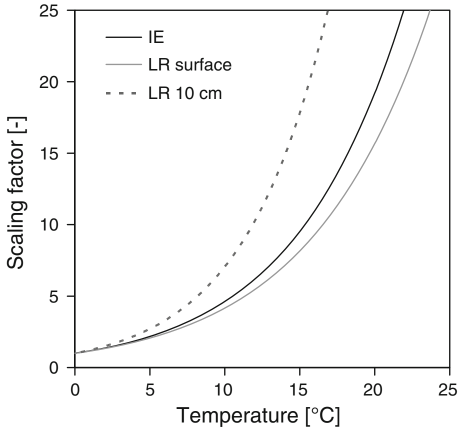

Fig. 7 Comparison of temperature response determined by inverse parameter estimation (IE) and the conventional linear regression method (LR) for different soil depths

method for estimating temperature sensitivity. The inversely estimated activation energy was 98 kJ mol^{-1} (Table 4, Fig. 7), which is in between the activation energy for soil surface temperature and temperature at 10 cm depth, as expected.

Summary and conclusions

The temperature and soil water content response of soil heterotrophic respiration are crucial for a reliable prediction of soil carbon dynamics. The direct determination of the temperature and soil water content response from field measurements is complicated by the interdependency of soil temperature and water, the quantitative and qualitative change of SOM, and the contribution of root respiration to measured soil respiration. Apparent response equations derived from relating measured CO_2 fluxes and temperature or water indicators (e.g. matric potential, water content, precipitation and evapotranspiration) may significantly differ from the intrinsic response. For example, the activation energy of the Arrhenius equation determined using the conventional regression method varied between 92 and 126 kJ mol^{-1} for the upper 10 cm of the soil profile. In this study, we determined the temperature and water response of soil heterotrophic respiration by means of inverse parameter estimation using the SOILCO2/RothC model. Due to the implementation of the RothC multi-pool carbon concept into the physically based transport model SOILCO2, temporal changes of temperature, water content, and the concentration and composition of SOM can be described in detail for the entire soil profile.

The inverse parameter estimation approach considered four widely used temperature response functions. The best prediction of measured CO_2 fluxes was obtained by a soil water content reduction function with an optimum at 62% water filled pore space and a temperature response equation according to the formulation of Parton et al. (1987). However, the commonly used Arrhenius equation provided similarly good results. The divergence of the fitted temperature response functions for temperatures above 25°C indicates that the fitted functions might not be reliable in this range. The excellent agreement between the temperature response functions for temperatures below 25°C is encouraging. The activation energy of the Arrhenius equation determined using inverse modelling was within the range of activation energies obtained from the conventional regression approach spanned over the soil profile. It was concluded that inverse parameter estimation is a promising alternative tool for the in situ determination of the temperature and soil water content response of soil respiration. Future synthetic model studies should investigate to what extent the inverse modelling approach can disentangle confounding factors that typically affect statistical estimates of the sensitivity of soil respiration to temperature and soil water content.

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