

# Separating soil CO<sub>2</sub> efflux into C-pool-specific decay rates via inverse analysis of soil incubation data

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**Abstract** Soil organic matter (SOM) is heterogeneous in structure and has been considered to consist of various pools with different intrinsic turnover rates. Although those pools have been conceptually expressed in models and analyzed according to soil physical and chemical properties, separation of SOM into component pools is still challenging. In this study, we conducted inverse analyses with data from a long-term (385 days) incubation experiment with two types of soil (from plant interspace and from underneath plants) to deconvolute soil carbon (C) efflux into different source pools. We analyzed the two datasets with one-, two- and three-pool models and used probability density functions as a criterion to judge the best model to fit the datasets. Our results indicated that soil C release trajectories over the 385 days of the incubation study were

best modeled with a two-pool C model. For both soil types, released C within the first 10 days of the incubation study originated from the labile pool. Decomposition of C in the recalcitrant pool was modeled to contribute to the total CO<sub>2</sub> efflux by 9–11 % at the beginning of the incubation. At the end of the experiment, 75–85 % of the initial soil organic carbon (SOC) was modeled to be released over the incubation period. Our modeling analysis also indicated that the labile C-pool in the soil underneath plants was larger than that in soil from interspace. This deconvolution analysis was based on information contained in incubation data to separate carbon pools and can facilitate integration of results from incubation experiments into ecosystem models with improved parameterization.

**Keywords** SOC · Labile C · Recalcitrant C ·  
Data assimilation · Parameter estimation

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## Introduction

Soils contain about two-thirds of all organic carbon (3,000 Pg C) that is stored in terrestrial ecosystems (Jobbágy and Jackson 2000) and yearly release  $98 \pm 11$  Pg C to the atmosphere (Bond-Lamberty and Thomson 2010). Total soil CO<sub>2</sub> efflux yearly exceeds the current rate of anthropogenic CO<sub>2</sub> emissions from deforestation and burning of fossil fuels by a factor of 10 (Solomon et al. 2007). These large numbers show that even small changes in soil C cycling are highly relevant to the global C cycle as soils have the potential to enhance or mitigate current increases in atmospheric CO<sub>2</sub>.

Total soil organic carbon (SOC) consists of different C-pools with intrinsic turnover rates ranging from less than a year to thousands of years (Amundson 2001; Trumbore

1997). Generally, soil organic carbon (SOC) is partitioned into at least three C-pools with different turnover times (e.g., Davidson and Janssens 2006; Parton et al. 1987; Trumbore 1997). SOM lability is defined by the decomposability of SOM by microbes and depends on chemical recalcitrance and physical protection of the soil (McLauchlan and Hobbie 2004). Each pool contributes to the total soil CO<sub>2</sub> efflux with availability of substrates varying during the course of an incubation study. The most active and therefore most easily decomposed C-pool can account for up to 20 % of the total SOC pool depending on soil type, vegetation cover, or geographical region (Trumbore 1997), but values are usually much lower (Haddix et al. 2011; McLauchlan and Hobbie 2004). This labile C-pool has a very short turnover time of a few days or a few weeks at most. The largest fraction of SOC (up to 80 %) is generally considered to be in an intermediate C-pool with turnover times of years to decades. This intermediate C-pool contains more complex structures that are less easily decomposable, either because of low litter quality or because some compounds are physically and chemically protected from fast decomposition (Davidson and Janssens 2006). The third C-pool can account for up to 50 % in organic poor soils and is often called the recalcitrant C-pool, as turnover times of this C-pool are estimated to be higher than 100 years and some of that C might persist in the soil for thousands of years (Trumbore 1997). Although SOC can be grouped into C-pools of different turnover times, there is a continuum between the pools, while strict separation between pools is impossible (Davidson and Janssens 2006; Parton et al. 1993; Paul et al. 2006; Schmidt et al. 2011). Separating C-pools with different turnover times from each other is challenging, but has been addressed in various studies and approaches. Physical fractionation is one of these approaches and uses differences in particle size and density of labile and recalcitrant fractions (Christensen 1992). Chemical fractionation includes the extraction of SOM in aqueous and acidic solutions in order to estimate the quality of the C-pools (for a review, see von Lützow et al. 2007). Both techniques are useful in separating C-pools with different turnover rates, with each method having its limitations. Fractionation of SOM has also been used to verify pool sizes that were determined through conceptual models (Motavalli et al. 1994; Zimmermann et al. 2007).

Soil incubation studies are advantageous to assess C decomposition rates of different C fractions, as there is usually no new input of organic material during the course of an incubation study and the labile C-pool is depleted without being replaced. Depending on the length of the incubation study, the labile C-pool will be completely decomposed and the measured soil CO<sub>2</sub> efflux originates from more stable C-pools. The advantage of soil incubation

studies is that treatment effects such as temperature can be applied isolated, factors such as pH, soil water content and nutrient supply can be controlled, and soils from different origins can be compared (Holland et al. 2000; Nadelhoffer 1990). Soil incubation studies that last longer than 100 days reduce the dominance of the labile C-pool and will show contributions of the more recalcitrant C-pools to the soil CO<sub>2</sub> efflux (von Lützow and Kögel-Knabner 2009). Therefore, to see changes in the contribution of the more recalcitrant C-pools to total soil CO<sub>2</sub> efflux, the length of an incubation study is the determining factor. Besides the duration of incubation studies, the size of the soil C-pool and the decomposability of the C-pool determine how much C will be decomposed during an incubation study.

Data assimilation is an approach to fuse diverse datasets into models to optimize parameter estimation and to allow for inferences from available data which are not directly observable, such as CO<sub>2</sub> efflux from C-pools of different turnover times (Wang et al. 2009; Zobitz et al. 2011). The data assimilation approach has been used several times for deconvolution of soil respiration rate into source components (Luo et al. 2001; Luo and Zhou 2010; Zhou et al. 2010). For example, Luo et al. (2001) deconvoluted soil respiration of a temperate forest ecosystem into C transfer processes and showed that fast cycling C processes such as root exudation are of minor importance for the whole ecosystem C cycle. Another deconvolution study partitioned soil respiration into autotrophic and heterotrophic components for understanding their differential responses to climate change (Zhou et al. 2010).

In this study, we conducted inverse analyses of data from long-term incubation experiments with two different soil types to deconvolute soil carbon efflux into different source pools. We used two soil types with different plant cover, as the availability and size of different C-pools is strongly affected by plant productivity (Hook et al. 1991). This data assimilation approach optimizes parameter estimation by introducing (1) predefined parameter ranges and (2) soil incubation datasets into the model. The objectives of this study were to model soil C dynamics of long-term incubation data to obtain soil CO<sub>2</sub> efflux rates of C-pools with different turnover times and to model C dynamics of various pools over the course of the incubation study. We hypothesize that optimal parameter estimation of more than one carbon pool depends on the quality of the dataset (measurement frequency) and on the length of the incubation study. We also hypothesize that a 385-day-long incubation time is not long enough to provide information to constrain parameters of a third, recalcitrant, C-pool. By using 1-pool, 2-pool, and 3-pool models, we will reveal which model best describes C dynamics of two different soils over the 385-day incubation period. Furthermore, this modeling approach will allow for detection of very small

differences between soils, and we hypothesize to see a larger labile C fraction in a soil that has more plant-derived organic C input.

## Materials and methods

### Incubation dataset

The dataset used in this study was obtained from an incubation study conducted in 2001 by Schaeffer et al. (unpublished). Soils for this incubation study were obtained from the Nevada Desert Free-Air CO<sub>2</sub> Enrichment (FACE) Facility (NDEF) which is 15 km north of Mercury, NV, USA (36°49'N, 115°55'W, elevation 965–970 m; Jordan et al. 1999). Soil was collected at three locations for each cover type in each of the six plots, and pooled according to cover type to generate four composited soil samples per plot. Soil samples were taken from the ambient CO<sub>2</sub> treatment under the dominant shrub (*Larrea tridentate*) and from between plants (interspace) to investigate differences in soils with different initial SOC pool size and a different long-term history in terms of fresh organic C input. We will refer to soil under *Larrea* as soil type ‘plant’ and to soil from plant interspace as soil type ‘interspace’ throughout the manuscript. Soils were sieved (2 mm) and 50 g dry weight of each soil type was placed in 5.3-cm-diameter × 5.0-cm-tall polyvinyl chloride cores, held by glassfiber filter paper taped to the bottom ( $n = 3$ ). Cores were placed inside a 1-L gas-tight jar equipped with a gas sampling port. Samples rested on glass marbles within the jar to allow air flow across the bottom of the cores. On days 1, 7, 19, 43, 84, 228, 315, and 385, 9 mL of gas were extracted from each jar into a pre-evacuated, gas-tight glass vial. After each gas sampling, four samples of ambient laboratory air were taken out before sealing the jars. Between sampling dates, samples were stored in the dark at 30 °C, and kept at constant moisture content (60 % of water holding capacity). Gas samples were analyzed for CO<sub>2</sub> on a Shimadzu 14A gas chromatograph (GC14-A; Dallas, TX, USA) equipped with thermal conductivity (CO<sub>2</sub>) detectors. Rates of CO<sub>2</sub>–C evolution (non-partitioned) were calculated as the CO<sub>2</sub> concentration over time, respectively, accounting for jar headspace, soil mass, and initial concentrations in laboratory air. Total initial organic C-pool size was obtained from Schaeffer et al. (2007) and accounted for 1.97 mg C g dry mass<sup>-1</sup> for the soil type ‘interspace’ and for 5.83 mg C g dry mass<sup>-1</sup> for the soil type ‘plant’. Soil CO<sub>2</sub> efflux from the incubation study was used for the C dynamics model to better estimate parameters of C decomposition of pools with different turnover time.

### C dynamics model

Total soil respiration was modeled using Eq. 1, with  $R$  being the sum of all respiration rates  $r_i$  from C-pools  $C_i$ . Pool specific respiration rates ( $r_i$ ) were modeled as the pool-specific decay rate ( $k_i$ ) times the total C-pool ( $C_{tot}$ ) times the partitioning coefficient of the specific pool to the total C-pool ( $f_i$ ). The change in carbon pool size for fraction  $i$  was modeled by a 1st order differential equation (Eq. 2) with C-pool  $i$  decaying at a temperature-dependent rate  $k_i$  over time ( $t$ ) multiplied by the total initial organic C-pool ( $C_{tot}$ ) times a partitioning coefficient ( $f_i$ ). The partitioning coefficient describes the portion of each C-pool to the total soil organic C-pool (Eq. 3) and the sum of all C-pools equals 1 (Eq. 4).

$$R = \sum_{i=1}^n r_i = \sum_{i=1}^n k_i C_{tot} f_i \quad (1)$$

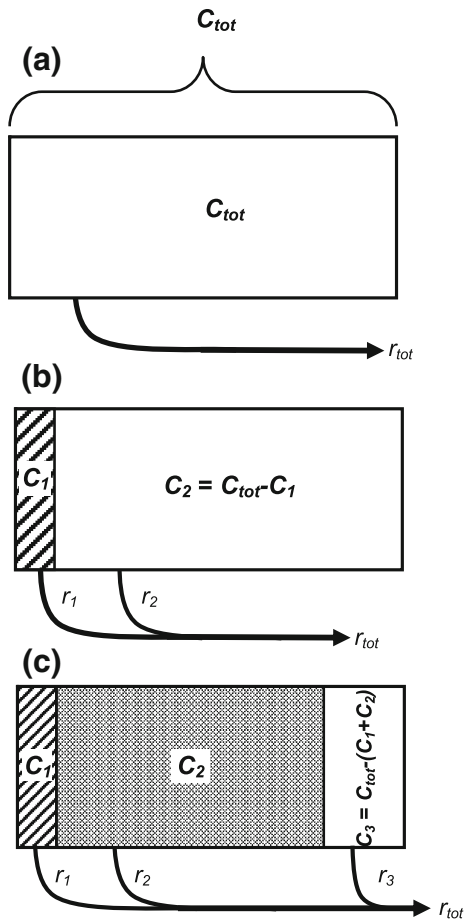
$$\frac{dC_i(t)}{dt} = -k_i C_{tot} f_i \quad (2)$$

$$f_i = \frac{C_i}{C_{tot}} \quad (3)$$

$$\sum_{i=1}^n f_i = 1 \quad (4)$$

For each soil type separately, we started to model respiration rates and soil C dynamics with a 1-pool model assuming that all C is in one total C-pool and therefore has the same turnover time (Fig. 1a). We then increased the number of C-pools in the 2-pool model (Fig. 1b) to two C-pools and finally to three C-pools in the 3-pool model (Fig. 1c). Depending on the number of C-pools, we obtained different respiration rates ( $r_i$ ) deriving from the corresponding C-pool ( $C_i$ , Fig. 1a–c). Total respiration rate ( $r_{tot}$ ) in the 1-pool model consisted of a single CO<sub>2</sub> efflux as there is only one C-pool. In the 2-pool model, total respiration rate was the sum of  $r_1 + r_2$  with  $r_1$  being the CO<sub>2</sub> efflux of the most active C-pool ( $C_1$ ) and  $r_2$  being the CO<sub>2</sub> efflux of a larger more stable C-pool ( $C_2$ ). In the 3-pool model,  $r_{tot}$  was the sum of  $r_1 + r_2 + r_3$  with  $r_1$  deriving from the most active C-pool ( $C_1$ ),  $r_2$  deriving from the intermediate C-pool ( $C_2$ ), and  $r_3$  originating from the most recalcitrant C-pool ( $C_3$ ).

To better model C-decomposition rates from different C-pools, we used data assimilation, which is the introduction of datasets (observed data) and prior knowledge of parameters to optimize parameter estimation. Parameters to estimate in this modeling study were decay rates ( $k_i$ ) and partitioning coefficients ( $f_i$ , Table 1).



**Fig. 1** Schematic depiction of the different soil C-pools for the soil C dynamics model. The *box* represents the total soil organic C-pool. **a** 1-pool model: total C is represented in 1-C-pool, **b** 2-pool model: total C is partitioned into a small labile C-pool ( $C_1$ ) and a large more stable C-pool ( $C_2$ ), **c** 3-pool model: total C is partitioned into three C-pools,  $C_1$  is the active C-pool,  $C_2$  intermediate C-pool, and  $C_3$  is the recalcitrant C-pool. Pool-specific respiration rates are shown as  $r_1$ ,  $r_2$ , and  $r_3$  with numbers being the same as for the C-pools;  $r_{tot}$  is the total respiration

#### Data assimilation

Bayesian probabilistic inversion was used to optimize parameters ( $p$ ) of the C dynamics models in this study. The inversion approach was developed by Xu et al. (2006) and is based on Bayes' theorem (Eq. 5), which states that the posterior probability density function (PPDF)  $P(p|Z)$  of model parameters ( $p$ ) can be obtained from prior knowledge of parameters, represented by a prior probability density function  $P(p)$ , and the information that is contained in the  $CO_2$  efflux dataset, represented by a likelihood function  $P(Z|p)$ .

$$P(p|Z) \propto P(Z|p)P(p). \quad (5)$$

To perform the Bayesian inversion, we first specified ranges (lower and upper limit, Table 1) of model

parameters according to literature values (Balesdent 1987; Craine et al. 2010; Fang et al. 2006; Trumbore 1997, 2000), assuming a uniform distribution over the specific parameter ranges. The likelihood function  $P(Z|p)$  (Eq. 6) was calculated with the assumption that errors between observed and modeled values followed a Gaussian distribution, where  $Z(t)$  denotes the data obtained from measurements,  $X(t)$  is the modeled value, and  $\sigma$  is the standard deviation of the observed  $CO_2$  efflux.

$$P(Z|p) \propto \exp \left\{ -\frac{1}{2\sigma^2} \sum_{t \in \text{obs}(Z_i)} [Z_i(t) - X_i(t)]^2 \right\} \quad (6)$$

Within the parameter space, the Metropolis–Hastings (M–H) algorithm, which is a Markov Chain Monte Carlo (MCMC) technique, was used to sample parameter sets that minimized the data-model error (Hastings 1970; Metropolis et al. 1953). The Metropolis–Hastings algorithm repeats two steps: a proposing step and a moving step (Xu et al. 2006). In the proposing step, the algorithm generates a new point  $p^{\text{new}}$  on the basis of the previously accepted point  $p^{(k-1)}$  with a proposal distribution  $P(p^{\text{new}}|p^{(k-1)})$  (Eq. 7).

$$p^{\text{new}} = p^{\text{old}} + d(p_{\text{Max}} - p_{\text{Min}})/D \quad (7)$$

In Eq. (7),  $p_{\text{max}}$  and  $p_{\text{min}}$  are the maximum and minimum values in the prior range of the given parameter,  $d$  is a random variable between  $-0.5$  and  $0.5$  with a uniform distribution, and  $D$  controls the proposing step size and was set to 7 for all three C-pool models. In each moving step, the new point  $p^{\text{new}}$  is tested against the Metropolis criterion (Xu et al. 2006) to examine if it should be accepted or rejected. If the ratio of the posterior probability densities at the new point  $p^{\text{new}}$ , and the previously accepted point  $p^{(k-1)}$  ( $p^{\text{new}}|p^{(k-1)}$ ) is larger than 1, the algorithm accepts the new point. If the ratio is less than 1, the algorithm rejects the point and takes another random step, still using the previously accepted point. The M–H algorithm was run 100,000 times for the 1-pool and 2-pool models and 300,000 times for the 3-pool model. Acceptance rate for parameter values was 21 % for the 1-pool model, 12 % for the 2-pool model, and 9 % for the 3-pool model.

Histograms of the series of samples were produced to display the distribution of the parameters within the parameter space. Maximum likelihood estimates (MLEs) of parameters ( $p_i$ ) were calculated by examining the parameter values corresponding to the peaks of marginal distributions and parameter means  $E(p_i)$  were calculated by:

$$E(p_i) = \frac{1}{k} \sum_{n=1}^k p_i^{(n)} \quad (8)$$

**Table 1** Prior ranges and maximum likelihood estimates of parameters for each C-pool model and each soil type

Parameters <sup>a</sup>	Lower limit	Upper limit	MLE <sub>plant</sub>	MLE <sub>interspace</sub>
1-pool model				
$k_1$	0.005	0.05	0.026	0.027
2-pool model				
$f_1$	0	0.2	0.137	0.118
$k_1$	0.1	0.7	0.359	0.507
$k_2$	0	0.01	$5.0 \times 10^{-3}$	$4.6 \times 10^{-3}$
3-pool model				
$f_1$	0	0.2	0.134	0.120
$f_2$	0.1	1.0	0.805	0.784
$k_1$	0.1	0.7	0.361	0.488
$k_2$	$1 \times 10^{-5}$	$1 \times 10^{-2}$	$5.4 \times 10^{-3}$	$5.4 \times 10^{-3}$
$k_3$	$1 \times 10^{-7}$	$1 \times 10^{-5}$	$5.0 \times 10^{-6b}$	$5.0 \times 10^{-6b}$

$k_i$  = pool specific decay rate ( $\text{day}^{-1}$ );  $f_i$  = C-pool partitioning coefficient

<sup>a</sup> Parameter ranges estimated according to Balesdent (1987), Trumbore (1997, 2000), Fang et al. (2006), Craine et al. (2010)

<sup>b</sup> Mean value

where  $k$  is the number of samples from the M–H algorithm and  $i = 1$  for the 1-pool model,  $i = 1, 2, 3$  for the 2-pool model, and  $i = 1, 2, \dots, 5$  for the 3-pool model. Parameter evaluation was used to decide how much information was contained in the data source (soil respiration) to model soil C dynamics in a 1-pool, 2-pool, or 3-pool model.

## Results

### Inversion analysis of soil C dynamics

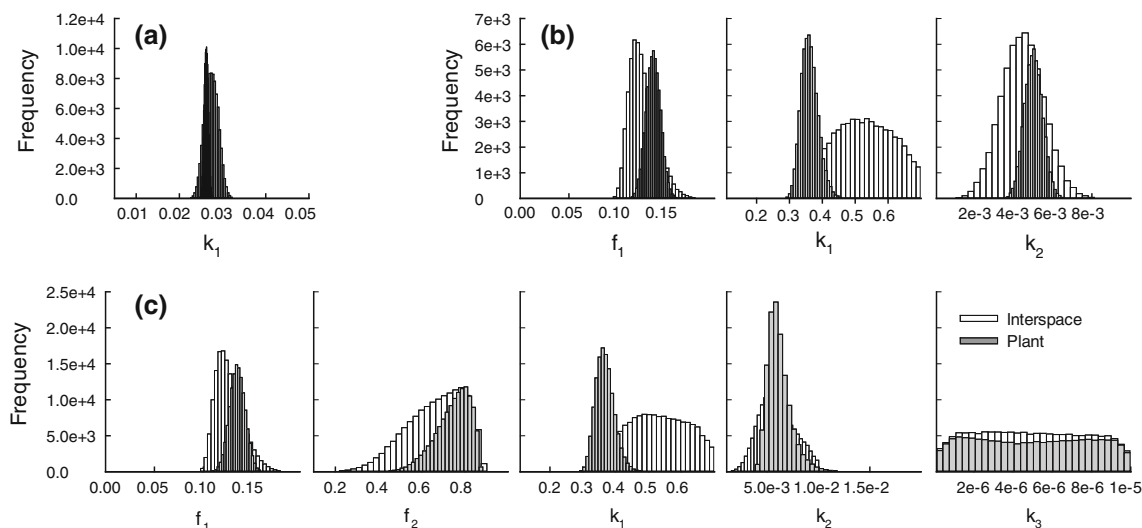
According to the shape of the posterior PDFs, the single parameter ( $k_1$ ) in the 1-pool model (Fig. 2a) was well constrained for both soil types. In the 2-pool model, all three parameters ( $f_1, k_1, k_2$ ; Fig. 2b) of both soil types were well constrained within their predetermined range although maximum likelihood estimates of the parameters differed between soil types (Table 1). Four out of five parameters were well constrained in the 3-pool model and only  $k_3$  was poorly constrained for both soil types. A maximum likelihood estimate (MLE) was calculated for each of the well-constrained parameters, while a mean value was calculated for the poorly constrained parameter. MLEs for  $k_1$  were very similar between the two soil types when a 1-pool model was used, but varied when a 2-pool or a 3-pool model was used. A slightly larger partitioning coefficient  $f_1$  for the soil type ‘plant’ indicates a 2 % larger labile pool. The smaller decomposition rate for the labile pool ( $k_1$ ) of

soil type ‘plant’ denotes a slightly higher residence time (residence time =  $1/k_1$ ) of 2.8 days rather than 1.9 days as for the soil type ‘interspace’. For both soil types, decay rates declined with increasing recalcitrance of the C-pools, and  $k_2$  in the 2-pool model was two orders of magnitude smaller than  $k_1$  (Table 1). Parameters of the 3-pool model were well constrained except for  $k_3$  (both soil types). The C-pool partitioning coefficient  $f_1$  in the 3-pool model explains that the active C-pool ( $C_1$ ) accounts for 12 % in the soil type ‘interspace’ and for 13.4 % in the soil type ‘plant’. The partitioning coefficient  $f_2$  stands for the size of the intermediate C-pool ( $C_2$ ), which accounts for 78 % in the soil type ‘interspace’ and for 80.5 % in the soil type ‘plant’. The recalcitrant C-pool ( $C_3$ ) is obtained by subtracting the total C-pool ( $C_{\text{tot}}$ ) minus the sum of the labile and intermediate C-pool, and accounts for 10 % in the soil type ‘interspace’ and for 6.1 % in the soil type ‘plant’ of the total organic C at the beginning of the incubation study (Table 1).

### C decomposition

Observed and modeled respiration rates are shown in Fig. 3 (only soil type ‘plant’ is shown since the patterns are similar for both soil types). The observed respiration rates were highest at the beginning of the incubation and sharply declined within the first 7 days and more moderately thereafter. The 1-pool model simulated one respiration rate, which was not as high as the observed respiration rate at the beginning of the incubation, and then declined smoothly over time (Fig. 3a). The 2-pool model simulated two respiration rates, with  $r_1$  being the respiration rate of the active C-pool ( $C_1$ ) and  $r_2$  being the respiration rate of the more recalcitrant C-pool ( $C_2$ , Fig. 3b). Total modeled respiration rate was composed mainly of  $r_1$  at the beginning of the incubation study, and after 7 days, both respiration rates were equally low. After day 7,  $r_1$  decreased to almost zero for the rest of the incubation study, whereas  $r_2$  remained at the same level although slightly decreasing over time. The sum of both respiration rates very well matched the observed values ( $r^2 = 0.998$ ; Fig. 3e). In the 3-pool model, we added a third respiration rate which represents the C-decomposition from the recalcitrant C-pool (Fig. 3c). This respiration rate was consistently low over the whole incubation period but still showed a slight decline over time. Adding a third C-pool and with that a third respiration rate did not improve the total modeled respiration rate for 385 days of incubation. Correlations of the observed respiration rate versus the total modeled respiration rate showed equally good fits for the 2-pool and 3-pool models ( $r^2 = 0.998$  for both models; Fig. 3e, f).





**Fig. 2** Frequency distribution of the posterior PDFs of all samples from five parallel runs for each parameter of both soil types for **a** 1-pool model, **b** 2-pool model, and **c** 3-pool model. The X-axis

shows the predetermined range of each parameter.  $k_i$  = pool specific decay rate in  $\text{mg C g}^{-1} \text{ soil day}^{-1}$ ;  $f_i$  = C-pool partitioning coefficient

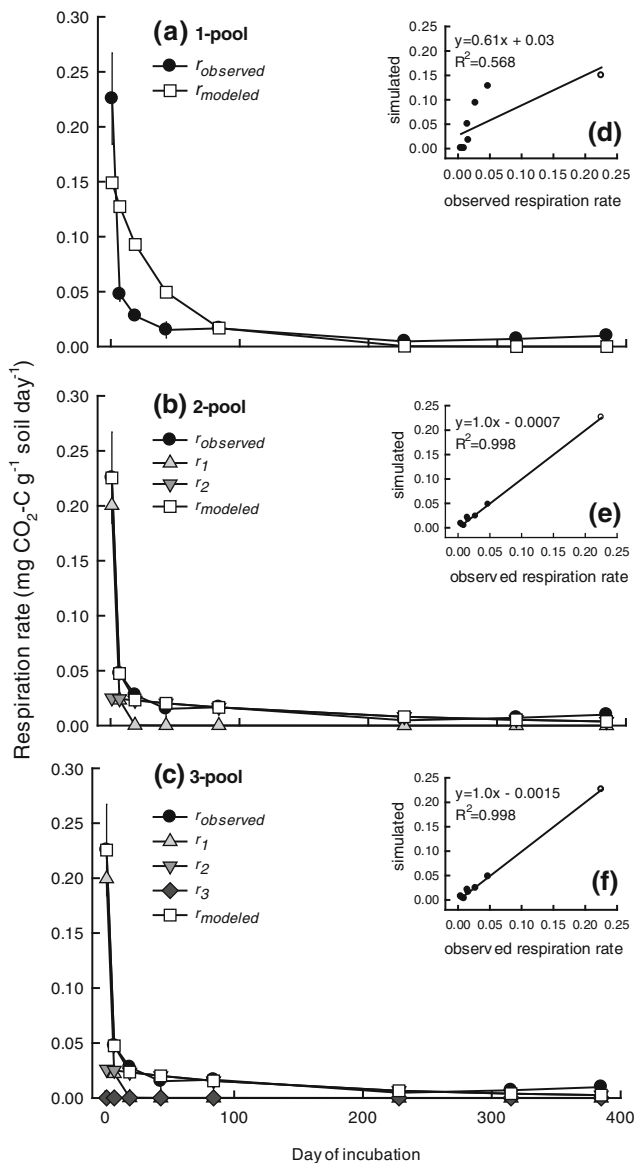
### C-pool dynamics

The dynamics of C-pool sizes with incubation days for each C-pool are presented in Fig. 4. For the 1-pool model, the total C-pool declined sharply over the incubation period and almost no C was left after 300 days of incubation for both soil types (Fig. 4a). In contrast, the 2-pool and 3-pool models showed a more moderate decline in total SOC. There was still 24 % (soil type ‘interspace’) and 14 % (soil type ‘plant’) of the total SOC left after 385 days of incubation (Fig. 4d). Both the 2-pool and 3-pool models revealed that most of the C was in the second pool ( $C_2$ ) and that the labile C-fraction ( $C_1$ ) was small and almost entirely depleted after 20 days (Fig. 4b). The patterns are similar for both soil types except that the decline in the total soil C was faster when the C-pool size was greater (76 % decline in C-pool size for the soil type ‘interspace’ vs. 86 % for the soil type ‘plant’).

In the 3-pool model, the fraction of the labile C-pool ( $C_1$ ) was the same as in the 2-pool model, but the rest of the C is separated into a large intermediate C-pool ( $C_2$ ) and a smaller, recalcitrant C-pool ( $C_3$ ). At the beginning of the incubation study,  $C_1$  accounted for 8 % (soil type ‘interspace’) and 10 % (soil type ‘plant’),  $C_2$  accounted for 70 and 77 % and  $C_3$  accounted for 22 and 13 % of the total SOC pool, respectively (Fig. 5). After 385 days of incubation, the ratios of individual C-pools to total SOC changed greatly (Fig. 5). Total SOC declined about 70 % (soil type ‘interspace’) and 80 % (soil type ‘plant’) over the entire incubation period and no C was left in the labile pool. The intermediate C-pool ( $C_2$ ) represented the largest C-pool in both soil types (70 % for soil type ‘interspace’

and 77 % for soil type ‘plant’) at day 1 of the incubation, but since more than 80 % of this C-pool was decomposed (Fig. 4f) during the course of the incubation, the recalcitrant C-pool ( $C_3$ ) accounted for the largest fraction after 385 days of incubation (71 vs. 61 %, respectively; Fig. 5).

We also calculated the contribution of each C-pool to the total respiration rate (Table 2). For the 1-pool model, all C that was decomposed came from the total C-pool, so there was no contribution to be calculated. But for the 2-pool and 3-pool models, we calculated the contribution of the labile C-pool ( $C_1$ ) to the total soil respiration to be 91 % for the soil type ‘interspace’ and 89 % for the soil type ‘plant’ at the first day of incubation. After 20 days, the labile C-pool contributed less than 1 % to the total respiration rate in the 2-pool model and all the C that was decomposed originated from the more stable C-pool ( $C_2$ ). Although, at the beginning of the incubation study, most of the C decomposed came from the labile C-pool, there was already a considerable contribution of the intermediate pool (9 % in soil type ‘interspace’ and 11 % in soil type ‘plant’) to the total respiration rate. In the 3-pool model, the contributions of the labile and intermediate C-pool ( $C_1$ ,  $C_2$ ) were the same as in the 2-pool model and the third C-pool ( $C_3$ ) only contributed about 0.1 % at the end of the incubation study. Although the pool size of the most recalcitrant C-pool was proportionally larger at the end of the incubation study (Fig. 5), it was still the intermediate pool that dominated the respiration rate after 385 days of incubation (Table 2). Differences in the contribution of individual C-pools to total respiration between the two soil types were found within the first 20 days of incubation (Table 2), both in the 2-pool and 3-pool models. Both



**Fig. 3** Observed and modeled respiration rates for the soil type ‘plant’ **a** 1-pool model, **b** 2-pool model, and **c** 3-pool model. Observed respiration rate is the mean  $\pm$  SD of three replicates and modeled respiration rate is the mean of five parallel runs.  $r_1$  is the respiration rate from the most labile pool,  $r_2$  derives from the more stable pool in the 2-pool model, and from the intermediate pool in the 3-pool model,  $r_3$  is the respiration rate from the recalcitrant pool. Modeled respiration rate ( $r_{\text{modeled}}$ ) is the sum of  $r_1 + r_2$  for the 2-pool model and the sum of  $r_1 + r_2 + r_3$  for the 3-pool model. Insets (**d–f**) show the correlation of the observed respiration rate against the simulated respiration rate

models show that after 20 days all of the carbon being decomposed originates from non-labile C-pools. At day 7 in the 3-pool model, the intermediate C-pool ( $C_2$ ) of the soil type ‘interspace’ contributed more (65.7 %) to the total respiration as the intermediate pool of the soil type ‘plant’ (53 %), since in the latter the contribution of the labile C-pool ( $C_1$ ) was larger (47 % compared to 34 %). This

difference disappeared after the first 20 days as the labile pool was depleted.

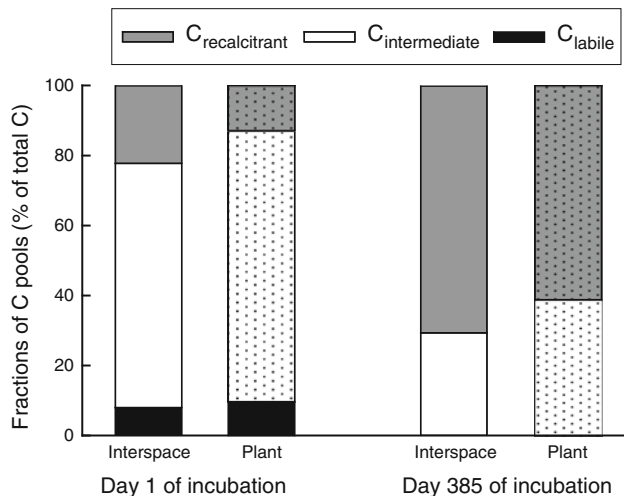
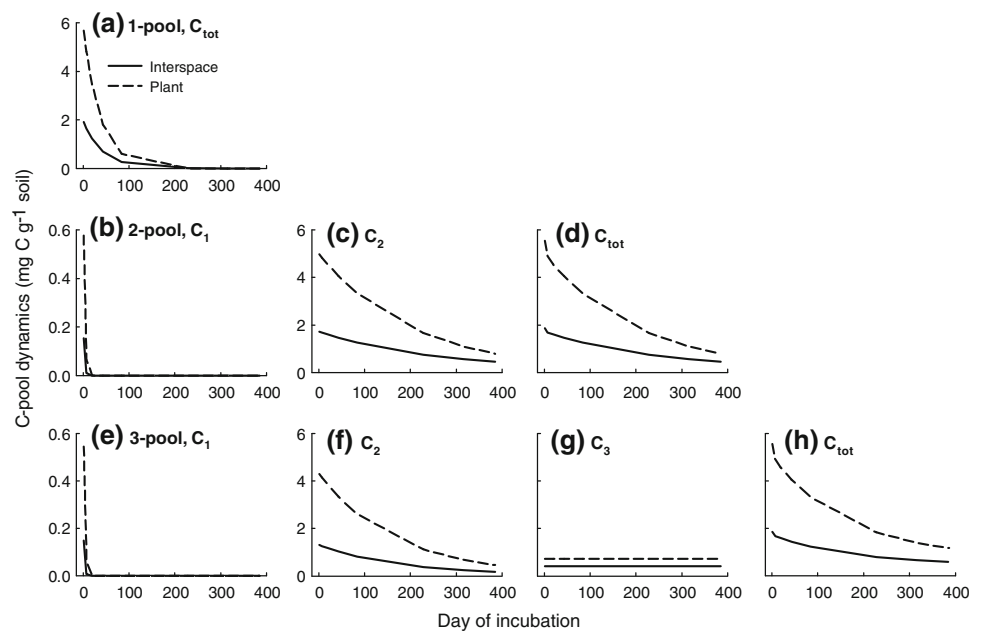
## Discussion

### Inverse analysis of soil incubation data

Incubation studies are a very useful way to measure decomposition rates of C-pools with different turnover times as there is no input of new carbon within the duration of an incubation study and the labile C-pool will be eventually depleted. In this study, we used a deconvolution approach to separate soil incubation data into different source pool respiration rates over time. Although SOM decomposition is very complex and includes various processes, it can be simulated relatively simply by using a first-order decay function (Jenkinson et al. 1990). Our model is a kinetic model and conceptually very similar to the CENTURY and RothC models which use 3–5 SOM pools (Jenkinson et al. 1990; Parton et al. 1987). All these conceptual models simulate SOM turnover over time and also describe decay processes to be best fit using more than one SOM pool. The CENTURY model simulates three soil organic matter fractions that represent (1) an active SOM fraction with a short turnover time of 1–5 years, (2) a slow SOM fraction with turnover times of 20–40 years, and (3) a passive SOM fraction that is chemically recalcitrant and has the longest turnover time with 200–500 years (Parton et al. 1987). The CENTURY model has been used amongst other things to detect changes in soil C storage with different land uses (Smith et al. 1997) or following climate change scenarios (Schimel et al. 1994). In the RothC model, SOM is partitioned into five pools that are classified as Decomposable Plant Material (DPM), Resistant Plant Material (RPM), Microbial Biomass (BIO), Humified Organic Matter (HUM), and an inert organic matter (IOM) fraction that is resistant to decomposition (Jenkinson 1990). Decomposition rates of these pools are set as constants (DPM = 10 year<sup>-1</sup>, RPM = 0.3 year<sup>-1</sup>, BIO = 0.66 year<sup>-1</sup>, HUM = 0.02 year<sup>-1</sup>) and are usually not altered when using the model. The RothC model was developed to simulate changes in SOC stocks with land use in different climatic regions (Smith et al. 1997). Both models can be used to describe long-term SOM dynamics in a range of ecosystems (Smith et al. 1997), whereas our model is used to describe C dynamics during incubation studies to estimate pool sizes and decay rates for C-pools with different turnover times. This inverse analysis is a new way to analyze incubation data and provides insights into C cycling of slow turnover pools.

In our study, we increased the number of C-pools with each model to find the right number of pools that could be

**Fig. 4** C-pool dynamics over the incubation period comparing both soil types (*dashed line* soil type ‘plant’, *solid line* soil type ‘interspace’) for the 1-, 2-, and 3-pool models.  $C_1$  represents the most active C-pool,  $C_2$  the more stable C-pool in the 2-pool model and the intermediate C-pool in the 3-pool model, and  $C_3$  is the recalcitrant C-pool.  $C_{tot}$  is the total C-pool and is the sum of  $C_1 + C_2$  in the 2-pool model and the sum of  $C_1 + C_2 + C_3$  in the 3-pool model. Please note the different scale on the y-axes in (b) and (e) to indicate the small labile C-pool ( $C_1$ )



**Fig. 5** Modeled fractions of C-pools (in % of total C) with different turnover times at day 1 and day 385 of the incubation for soil type ‘interspace’ (*no pattern*) and soil type ‘plant’ (*dotted pattern*)

modeled by the used set of incubation data without ignoring the law of parsimony. Apparently, SOM is not represented by a single C-pool, which becomes even more obvious when trying to fit decomposition rates of incubation studies that lasted longer than just a few days or weeks (Kätterer et al. 1998; Knorr et al. 2005). A 2-pool model fitted the incubation data really well and there was no improvement in the fit when a 3-pool model was used. This suggests that the incubation data did not provide enough information to perfectly model the decay rate of a third pool, as respiration rates were dominated by the labile pool at the beginning of the incubation study and then by the intermediate pool. In order to simulate decay rates of the

recalcitrant C-pool, we need long-term studies that last for much more than a few months. The data used in this incubation study were obtained from a 385-day incubation study and are considered to be long-term incubation data but still did not provide enough information to constrain parameters of the recalcitrant pool well. We could still determine the size of the third pool as it is calculated by the difference of the total C-pool and the sum of the labile and intermediate pool. But a poorly constrained parameter ( $k_3$ ) could not be used to quantify a maximum likelihood estimate, while the mean value over the whole parameter range calculated instead was not very indicative of the exact decomposition rate for the recalcitrant C-pool. Parameter distributions allowed for calculating MLE while parameter uncertainties could be assessed from confidence intervals (Xu et al. 2006). For the poorly-constrained parameter  $k_3$  in the 3-pool model, the parameter uncertainty was very large as the parameter could take any value within the parameter space.

Inverse analysis is a useful and powerful technique as it takes advantage of information contained in the data, model structure, and prior knowledge about parameters (Raupach et al. 2005). Several other studies have used inverse analysis to evaluate parameters of C dynamics in order to estimate model parameters that cannot be directly obtained from experimental data (Wu et al. 2009; Xu et al. 2006; Zhou et al. 2010).

Inverse estimation of C-pools has been performed by Scharnagl et al. (2010) applying synthetically generated mineralization rates using the RothC model. They described a 900-day incubation study as sufficient to optimally constrain parameters of all carbon pools in the RothC



**Table 2** Contribution (in %) of each C-pool to the total respiration rate for the 2-pool and 3-pool models for both soil types

Days	Interspace			Plant		
	C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>	C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>
<b>2-pool model</b>						
1	90.9	9.1		88.9	11.1	
7	33.5	66.5		48.8	51.2	
19	0.3	99.7		1.4	98.6	
43	0	100		0	100	
84	0	100		0	100	
228	0	100		0	100	
315	0	100		0	100	
385	0	100		0	100	
<b>3-pool model</b>						
1	91.1	8.9	<0.1	88.4	11.6	<0.1
7	34.3	65.7	<0.1	47.0	53.0	<0.1
19	0.3	99.7	<0.1	1.3	98.7	<0.1
43	0	100	<0.1	0	100	<0.1
84	0	100	<0.1	0	100	<0.1
228	0	99.9	0.1	0	99.9	0.1
315	0	99.8	0.2	0	99.9	0.1
385	0	99.8	0.2	0	99.9	0.1

model. Unlike in our study, they used an equal amount of measurements over the whole incubation period which likely helped constrain more recalcitrant C-pools. Although decomposition rates stabilize after a while, giving evidence for a slow but constant respiration rate of the recalcitrant C-pool (Dijkstra et al. 2005; Townsend et al. 1997), there is still considerable change over time that cannot be detected when measurements are taken within large timespans. In general, parameters that describe fast processes, such as C transfer from nonwoody biomass to metabolic or structural litter, are identified the best, as has been described in various other studies (Braswell et al. 2005; Wu et al. 2009; Xu et al. 2006). Decay rates of the recalcitrant C-pool describe a very slow process and, since incubation studies do usually not last very long, not enough information is provided by those datasets.

#### C-pool sizes of soils with different turnover times

Total SOC consists of C-pools with different chemical compositions, decomposabilities, and turnover times (Trumbore 1997). Various approaches have been developed to separate and assess different soil C fractions (Christensen 1992; von Lützwow et al. 2007). Chemical fractionation methods fractionate SOM according to their solubility, hydrolysability, and resistance to oxidation (von Lützwow et al. 2007). In chemical fractionation, different

extractants are used to obtain the most labile C-pool, ranging from cold or hot water to aqueous solutions of different ionic strength to simulate the soil solution (von Lützwow et al. 2007). Humic substances on the other hand belong to the recalcitrant C-pool, and most of them can be extracted best with alkaline solutions, preferably a mix of NaOH and Na<sub>4</sub>P<sub>2</sub>O<sub>7</sub> (Balesdent 1987). Alkanes and fatty acids can be extracted using repeated *n*-hexanes (Hayes 1985), and hemicelluloses and cellulose are extracted by acid hydrolysis, either HCl or H<sub>2</sub>SO<sub>4</sub> (Van Soest and Wine 1967). With all these chemical fractionation methods, SOM can be separated into functionally different pools, but those SOM pools are not homogenous in turnover time. In contrast, conceptual multi-C-pool turnover models are based on pool-specific turnover times and pool sizes. In this study, we also applied a conceptual model and additionally used the information that was contained in incubation data to quantify pool fractions. Turnover rates estimated by the model presented here combine SOM pools with homogeneous decay behavior but functionally different fractions.

Using inverse analysis to deconvolute incubation data into pool-specific decay rates not only allows for estimating respiration rates of pools with different turnover times but also allows the determination of pool sizes and their dynamics over the course of an incubation study. The intrinsic C-pool size is one of the most important factors for the magnitude of the C decomposition rate at the beginning of an incubation study. CO<sub>2</sub> efflux in the first few days of an incubation study is dependent on the size of the active pool (Paul et al. 2006), and mean residence times are calculated as the inverse of turnover rates (MRT = 1/*k*). Labile C-pools accounted for 10–13 % of the total SOC and had a turnover time of 2–3 days, which is in good agreement with previous studies (Pendall and King 2007). Although the soils were homogenized before being incubated, we rule out a large contribution of non-labile C in the first few days, as the lack of soil structure (aggregation), high sand content, and low organic matter content of these sandy soils suggest that the amount of physically protected organic matter (either in aggregates or mineral-bound) is relatively low.

MRTs of the intermediate pool in the 2-pool model was a little more than half a year, which seems very short compared to other studies (Paul et al. 2006; Pendall and King 2007). However, as the intermediate and recalcitrant pool were lumped together in the 2-pool model, it is not surprising that the MRT is so short, as decomposition rates were completely dominated by the intermediate C-pool. For the 3-pool model, we could not exactly define the MRT of the recalcitrant C-pool as the parameter was poorly constrained, but MRT would be between many years to thousands of years considering the initial parameter range. Paul et al. (2006) even declared that incubation data are

generally insufficient to estimate the size and turnover rate of the recalcitrant pool. Good estimates on the turnover rate of the recalcitrant C-pool also depend greatly on the quality and length of an incubation study, and it cannot be generally ruled out that incubation studies do not provide enough information for good estimation of the recalcitrant C-pool. Generally, frequent measurements even after the initial decline in respiration rate, should be considered to improve the detection limit of small differences in the more recalcitrant C-pools. For better parameter estimation of the intermediate and recalcitrant C-pools, we recommend long-term incubation studies to last for a few years, although results will depend on soil quality and incubation temperature. It should also be noted here that MRTs of C-pools calculated from incubation studies are often calculated under optimal temperature and moisture conditions for microbial activity, and turnover times in field conditions might be slightly lower. Nevertheless, this deconvolution study of long-term incubation data gives important information on C-pool sizes and their relative degradability.

We calculated a very low contribution of the recalcitrant C-pool to the total soil C efflux, but, after 230 days, the contribution of the recalcitrant C-pool became apparent, although it stayed constant over the rest of the incubation period. If the incubation study had continued much longer, the contribution of the recalcitrant C-pool would have become more and more important. This clearly shows that predictions of the recalcitrant C-pool can be better made when incubation studies go on for more than a year.

#### Comparison of C-pool dynamics between two soils

The percentage of carbon respired during an incubation study is negatively correlated with initial soil C concentration (Frank and Groffman 1998). Frank and Groffman (1998) showed that, during a 28-week-long incubation study, more than 50 % of the carbon can be respired when the initial carbon concentration is below 1 %. The soils used in this incubation study had low initial carbon concentrations (0.19 and 0.58 %), and high proportions of total carbon being decomposed are plausible. Soils at juxtaposed sites have carbonate concentrations from 16 to 30 %, and it has been questioned before that in arid soils some of the carbon being released might originate from inorganic sources (Billings et al. 2004) and therefore confound total C release from organic sources. A high contribution of inorganic carbon to the measured CO<sub>2</sub> efflux in this incubation data seems to be most possible for the first measurement point when  $\delta^{13}\text{C}$  values were slightly less than that of bulk soil (unpublished data), which indicates carbonate precipitation and carbonate contribution to CO<sub>2</sub> efflux (Mermut et al. 2000). Nevertheless, we assume that, for the incubation data used in

this study, most of the carbon being released originates from organic sources.

Since neither soil received any new C input during the incubation study, we were able to detect differences in size and dynamics of the labile versus the more recalcitrant C-pools. As expected, the labile pool from the soil type 'plant' was larger than from the soil type 'interspace', as fresh carbon added (in the field, not during the incubation study) increased the size of the easily decomposable carbon which had been previously described in a field manipulation study at the same site (Schaeffer et al. 2003). The largest difference in pool size was found in the intermediate C-pool in the 2-pool and 3-pool models. Soil type 'plant' had a 60 % larger intermediate C-pool than soil type 'interspace'. In agreement with the pool size, the decomposition rate was also higher in the soil type 'plant' than in the soil type 'interspace', but both decomposition rates aligned after 200 days of incubation, indicating that the more labile fractions had been depleted. Other studies using desert soil have described the same pattern that more C input through biomass resulted in higher decomposition rates, although those incubations only lasted for little more than a month and could not detect differences in the less labile C-pools (Nunez et al. 2001; Su et al. 2004). Soil-specific differences revealed that the recalcitrant C-pool in the soil type 'interspace' became the largest fraction of the total soil C-pool after only 200 days of incubation compared to 300 days of incubation for the soil type 'plant' (Fig. 4f, g). These small differences are easily detectable using the modeling approach and reveal information that is otherwise not detectable. The main difference between the two soils is the lack of fresh organic input in the field for the soil type 'interspace' compared to fresh litter input for the soil type 'plant'. Both soils have similar C content and classify as mineral soils and yet there are distinct differences in C dynamics between the soils. The purpose of using these two soils was that both were sampled and incubated in the same procedure but still had a different history of organic C input, which gives insights into the C dynamics of different soil types that are not biased by varying incubation procedures. Using both soils revealed that even small differences between soils can be detected when using this modeling approach, and hence inverse analysis of incubation data is well suited for more contrasting soils such as organic versus mineral soils or soils of different ecosystem types.

In this deconvolution analysis, the contribution of the labile pool dominated the CO<sub>2</sub> efflux to 90 % at the beginning of the incubation but was outplayed by the more stable fractions after only a few days. This reflects a rapid change from labile to recalcitrant C and has been demonstrated in previous studies (Pendall and King 2007; Townsend et al. 1997). During the rest of the incubation

study, the intermediate C-pool contributed most to the total C efflux, and only after more than 200 days did the contribution of the recalcitrant pool become measureable. To account for contributions of labile and intermediate C-pools to the total respiration, stable isotopic signatures of evolved CO<sub>2</sub> have been shown to provide very good results (Pendall and King 2007; Townsend et al. 1997). Townsend et al. (1997) used stable isotopes for sites where a shift in vegetation from forest to pasture occurred and with it a change in the photosynthetic pathway (soils under C<sub>4</sub> grasses are enriched in <sup>13</sup>C compared to soil from C<sub>3</sub> forest). Their results revealed that δ<sup>13</sup>C values for CO<sub>2</sub> efflux significantly decreased between days 7 and 120, which explains that more C was forest-derived (forest carbon is lighter in <sup>13</sup>C). These results nicely show that older carbon (forest-derived) increasingly contributed to decomposition rates with time in this 225-day-long incubation.

## Conclusion

Inverse analysis of long-term incubation studies enables the determining of the size and turnover time of different C-pools and is therefore a very powerful technique to detect changes in C cycling of slow turnover pools. The analysis also showed that differences in C-pool dynamics between soils due to varying initial C content can be easily detected. Furthermore, this modeling approach can be used to analyze C dynamics of soil incubations with different protocols, treatments, soil types, vegetation, and durations. Using this modeling approach to analyze incubation data conducted at different temperatures will reveal information to calculate temperature sensitivity of C-pools with different turnover. Better parameterization with this inverse analysis allows for the obtaining of more precise values for C-pool sizes and decay rates of different source pools. These parameters can then be incorporated into ecosystem models and will help improve estimation of soil C cycling. A 2-pool model best fit decomposition data of this 385-day-long incubation dataset which clearly shows that high quality long-term incubation datasets are needed in order to provide enough information to constrain parameters of C-pools with long mean residence times. The success of a deconvolution study always depends on the amount and quality of a dataset (Luo et al. 2001; Wang et al. 2009), and to make sure that incubation studies are not limited to reveal information of only more labile C-pools, we need long long-term studies of many years.

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**Conflict of interest** The authors declare that they have no conflict of interest.

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