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Information content of incubation experiments

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Information content of incubation experiments for inverse estimation of pools sizes in the Rothamsted carbon model: a Bayesian approach

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Abstract

Turnover of soil organic matter (SOM) is usually described with multi-compartment models. A model compartment (or pool) contains all carbon compounds with similar functional properties, such as decomposition rate and partitioning of decomposition products. These functionally defined carbon pools do not necessarily correspond to measurable (SOC) fractions in real practice. This not only impairs our ability to rigorously evaluate SOC models, but also makes it difficult to derive accurate initial states. In this study, we test the usefulness and applicability of inverse modeling to derive the various carbon pool sizes in the Rothamsted carbon model (ROTHC) using observed mineralization rate data during incubation of soil samples in the laboratory. In the last decade, inverse modeling has found widespread application and use for environmental model calibration, but this methodology has not yet been tested for assessing carbon pools in multi-compartment SOC models. To appropriately consider data and model uncertainty we consider a Bayesian approach using the recently developed DiffeRential Evolution Adaptive Metropolis (DREAM) algorithm. This Markov Chain Monte Carlo (MCMC) scheme derives the posterior probability density distribution of the initial pool sizes at the start of incubation from measured mineralization rates. Our results show that measured mineralization rates generally provide sufficient information to reliably estimate the sizes of all active carbon pools in the ROTHC model. However, for soils with slow and intermediate carbon turnover an excessively long incubation time is required to appropriately constrain all carbon pools. The explicit use of prior information on microbial biomass provides a way forward to significantly reduce uncertainty and required duration of incubation. Our illustrative case studies show how Bayesian inverse modeling can be used to provide important insights into the information content of incubation experiments for assessing SOC turnover and dynamics.

1 Introduction

A substantial part of the global carbon cycle occurs in the pedosphere. The upper meter of the soils of the world is estimated to contain 1500 Pg organic C (Batjes, 1996), which is approximately twofold the amount of carbon in the atmosphere and threefold
⁵ that stored in living plant material (Prentice et al., 2001). The link between terrestrial carbon cycling and climate change has recently received much attention because the pedosphere has the potential to either amplify or dampen global warming (e.g. Friedlingstein et al., 2006; Heimann and Reichstein, 2008). Moreover, it has long been recognized that SOM levels exert strong influence on the physical and chemical prop-
¹⁰ erties of soils, and consequently, determine soil productivity and its functioning as an ecosystem. Both fields of science demand for reliable modeling of soil organic carbon (SOC) dynamics.

SOM turnover is usually described with multi-compartment models. The model compartments (or pools) are generally defined by functional properties such as decom-
¹⁵ position rate, input and output pathways, and partitioning of decomposition products. These models have been successfully applied for simulating total soil organic carbon (SOC) levels observed in long-term field experiments (Smith et al., 1997). However, a major drawback of these models is that their functionally defined compartments do not necessarily correspond to measurable SOM fractions in real practice (e.g. Christensen,
²⁰ 1996; Elliott et al., 1996; Cambardella, 1998; Arah and Gaunt, 2001). The ongoing difficulty with direct measurement of the various carbon pools not only impairs our ability to rigorously evaluate SOM models, but also downplays the utility of these models for predictive purposes. Moreover, when using SOC models to understand and predict carbon dynamics in soils, we are faced with the problem of setting the initial pool sizes.
²⁵ In recent years, the Rothamsted carbon model (ROTHC, Coleman and Jenkinson, 1999) has found widespread application and use to study SOC dynamics. Several studies have developed fractionation procedures that yield SOC fractions which match as closely and consistently as possible the various pools considered in ROTHC (Jenk-

inson et al., 1992; Balesdent, 1996; Skjemstad et al., 2001; Ludwig et al., 2003; Skjemstad et al., 2004; Zimmermann et al., 2007). Notwithstanding this progress made, we believe that this approach of "measuring the modelable" (Elliott et al., 1996) is subject to considerable uncertainty and debate. For instance, Smith et al. (2002) pointed
5 out that, to be equivalent to a model pool, a measured fraction must be both unique (i.e. isolating all SOM pertaining to a conceptual pool) and non-composite (i.e. isolating SOM from one conceptual pool only). SOM fractionation is generally based on physical or chemical properties, or both. But it seems questionable if these properties alone, or a combination thereof, can be used to isolate unique and non-composite SOM fractions
10 that exhibit similar behavior and fate as the individual carbon pools defined in ROTHC. In a recent review on SOM fractionation methods and their relevance for modeling, von Lützow et al. (2007) concluded that only the microbial biomass and the light fraction (SOM that is not firmly associated with soil minerals and consists mostly of plant residues) can be reliably isolated. They argue that the currently available fractionation
15 techniques are not specific enough with regard to SOM stabilization mechanisms, and therefore, do not yield functional pools with homogeneous decomposition rates. This might explain why the opposite strategy of "modeling the measurable" (Elliott et al., 1996) – that is, building mathematical models based on measurable SOM fractions – has not yet found its way into standard modeling practice.
20   In this paper, we test the usefulness and applicability of inverse modeling for assessing carbon pools in the ROTHC model using data of measured mineralization rates during incubation of soil samples in the laboratory. Inverse modeling is arguably the most appropriate way of assessing the properties of the various carbon pools (Molina et al., 1994). This inverse approach, however has not been tested yet using a state-of-the-
25 art multi-compartment model. Here, we used a synthetic time series of mineralization rates generated with the ROTHC model to inversely estimate the posterior probability density distributions of the individual pool sizes in the ROTHC model at the beginning of the incubation experiment. To appropriately treat model and mineralization rate data uncertainty, we consider a Bayesian approach with the recently developed DiffeRential

Evolution Adaptive Metropolis (DREAM) algorithm (Vrugt et al., 2008, 2009). We explicitly address the following questions: (i) Do incubation experiments provide sufficient information to reliably estimate all carbon pools in ROTHC, especially those pools with intermediate and slow turnover? (ii) What length of incubation is required to appropriately constrain all pools? (iii) Would prior information on microbial biomass C reduce uncertainty of carbon pool size estimates?

2 Methods

2.1 Model description

A schematic overview of the Rothamsted carbon model (ROTHC, Coleman and Jenkinson, 1999) appears in Fig. 1. The ROTHC model has four active pools: decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO) and humified organic matter (HUM). Each pool is decomposed on its own, characteristic rate (Tab. 1). Decomposition rate constants were derived from field experiments with ^{14}C labeled plant material and ^{15}N labeled microbial biomass, as well as using data of total SOC from long-term field experiments at Rothamsted (Jenkinson et al., 1992). These rate constants are typically held constant when applying the model to other conditions. The mass balance of the active pools, c (g C kg^{-1} soil), is described with the relatively simple ordinary partial differential equation:

$$\frac{dc}{dt} = -k^* c + s \tag{1}$$

where t (year) is time, k^* (year^{-1}) denote the actual decomposition rates, and s (g C kg^{-1} soil year^{-1}) are inputs from organic material or other compartments. The actual decomposition rate k^* is modeled as a multiplicative product of the intrinsic decomposition rate constant k and three different reduction functions (dimensionless)

accounting for soil temperature, $f_1(T)$, soil moisture, $f_2(\theta)$, and soil cover, $f_3(\gamma)$:

$$k^* = f_1(T)\, f_2(\theta)\, f_3(\gamma)\, k \qquad\qquad (2)$$

The incoming plant material is partitioned between DPM and RPM in a ratio that depends on vegetation type, p_1(vegetation). The decomposition process releases part of the carbon as CO_2 to the atmosphere and distributes the remaining carbon between the BIO and HUM pools. The proportion of carbon that is mineralized, p_2(clay), depends on the clay content of the soil, while the ratio between carbon feed into BIO and into HUM, p_3, is fixed. A detailed description of the rate modifying functions and partitioning coefficients appears in Coleman and Jenkinson (1999), and so will not be repeated here. In addition to the four active pools (DPM, RPM, BIO and HUM), the ROTHC model also contains a fifth pool that is made up of inert organic matter (IOM). This pool is resistant to microbial decomposition and does not receive any carbon from the four other pools or other sources. It is assumed that the carbon in the IOM pool is of geological rather than pedological age, implying that it contains virtually no [14]C. The introduction of the IOM pool was necessary to match the ^{14}C signature of the soil, which usually indicates the presence of some small amount of very old carbon (Jenkinson et al., 1992). In all our calculations, we use a MATLAB implementation of the ROTHC model with an explicit Runge-Kutta solution scheme to solve for the system of ordinary diffeRential equations (Shampine and Reichelt, 1997).

2.2 Incubation experiment

We generated a time series of synthetic mineralization rates using the ROTHC model with values of the initial pool sizes and model parameters listed in Table 1. The initial pool sizes were obtained from a simulation of the long-term Broadbalk wheat experiment following the procedure and input data given in Jenkinson et al. (1992). The incubation temperature was set to 20 ˚C. The soil moisture during incubation was assumed to be at an "optimal" level and the soil cover was set to "bare". We assumed that measurements were taken on day 1, 7, 14, 21 and 28 of incubation and after that

on every 14th day till termination of the experiment. We investigated the information content of mineralization rate data for three different lengths of incubation. These include experiments that last 300, 600, and 900 days. Before using the synthetic data in our analysis, simulated mineralization rates were corrupted with a normally distributed random error to explicitly consider the presence of measurement error occuring in real practice. To obtain a realistic estimate of the measurement error, we used a real data set of mineralization rate measurements conducted with an automated respirometer. In Fig. 2 we plotted the standard deviation of observed mineralization rate against its mean measured value using 8 different samples. The data demonstrate that the measurement error increases at larger mineralization rates. To use this information in our Bayesian analysis, we fitted a straight line through the data with intercept 0.00014 and slope 0.019 $g C kg^{-1} soil day^{-1}$, and used this relationship to estimate the measurement error, σ, as function of observed mineralization rates. We further assumed that each observation is repeated $R=12$ times, the maximum number of repetitions possible within 24 h with our respirometer setup. From these 12 realizations, the mean and the standard deviation of the mineralization rate is calculated. We used the same realization of measurement errors for all experiments to ensure that differences in pool size estimates observed between the various experimental designs tested cannot be attributed to different realizations of the measurement error. Following Ellert and Bettany (1988) and Hess and Schmidt (1995) we use rates of mineralization rather than cumulative amounts to obtain realistic estimates of parameter uncertainty.

2.3 Inverse modeling

To help describe the inverse method utilized herein, lets denote the ROTHC model with the symbol M that simulates n mineralization rates $R=\{R_1, \ldots, R_n\}$ using the initial state variables S, with measured forcing variables $\hat{F}$, and model parameters P:

$$R = M(S, \hat{F}, P) \tag{3}$$

where the initial state of the SOC system S is defined by the sizes of the various pools at the start of the ROTHC simulation. The forcing variables $\hat{F}$ include observed soil temperature and soil moisture. Finally, the model parameters P consist of decomposition rate constants, rate modifying factors and partitioning coefficients.

5 Inverse modeling is a general method for estimating the arguments of M by minimizing some predefined measure of the residual vector $\boldsymbol{\varepsilon} = \{\varepsilon_1, \ldots, \varepsilon_n\}$. The residuals are defined by the differences between simulated variables R and corresponding measurements $\hat{R} = \{\hat{R}_1, \ldots, \hat{R}_n\}$:

$$\varepsilon_i(S|\hat{F}, P, \hat{R}_i) = R_i(S|\hat{F}, P) - \hat{R}_i \qquad i = 1, \ldots, n \tag{4}$$

10 The closer the residuals are to zero, the better the model represents the observational data. However, because of errors in observed forcing variables $\hat{F}$, structural inadequacies in the model that cause error in the simulated variables R, errors in the response variable measurements $\hat{R}$, and uncertainty in the model parameters P, the residuals are not expected to go to zero. Note that our use of inverse modeling in this paper is

15 rather different than typical implementations of this methodology that focus on estimating model parameters without recourse to considering initial state variables.

A popular measure that is commonly minimized during inverse modeling is weighted least squares:

$$\Phi(S|\hat{F}, P, \hat{R}) = \sum_{i=1}^{n} \left(\frac{\varepsilon_i(S|\hat{F}, P, \hat{R}_i)^2}{\sigma_i^2} \right) \tag{5}$$

20 where σ_i^2 is the variance of the ith response variable measurement. For models that are nonlinear in their estimated arguments, the minimum of $\Phi(S|\hat{F}, P, \hat{R})$ can neither be found by analytical evaluation nor by analytical approximation. Various numerical optimization methods have therefore been developed during the past decades to efficiently minimize this measure for multi-dimensional search spaces. Unfortunately, such algo-

25 rithms only provide an estimate of the best values of the estimated arguments. This

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would suffice in many practical applications, yet it would also be desirable to have an estimate of their underlying probability density function (pdf). This distribution will help assess the information content of the measured variables and help generate predictive distributions of R.

5   One approach to estimate uncertainty of state variables, parameters and model predictions is by adopting a Bayesian framework. In this approach, the estimated arguments are treated as probabilistic variables having a joint posterior pdf $p(S|\hat{F}, P, \hat{R})$. The posterior pdf summarizes what is known about the estimands given the measurements and prior information. If we assume that the measurement errors are independent and normally distributed with individual variance σ_i^2, the posterior pdf takes the following form:

$$p(S|\hat{F}, P, \hat{R}) \propto p(S) \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{\varepsilon_i(S|\hat{F}, P, \hat{R}_i)^2}{2\sigma_i^2}\right) \tag{6}$$

where $p(S)$ signifies the prior pdf of S. It summarizes the information on S before any measurements are available. In many applications of Bayesian statistics prior knowledge about the estimands is typically vague. In that case a uniform (non-informative) prior distribution is usually imposed. The Bayesian framework of statistical inference and prediction offers several important advantages over the classical frequentist approach. A detailed description and overview of both approaches is found in Reichert and Omlin (1997) and Omlin and Reichert (1999) and is beyond the scope of the current paper.

Unfortunately, for most practical problems the posterior pdf in Eq. (6) cannot be obtained by analytical means nor by analytical approximation. We therefore resort to iterative approximation methods such as Markov chain Monte Carlo (MCMC) sampling to generate a sample from the posterior pdf. The basis of the MCMC method is a Markov chain that generates a random walk through the search space with stable frequency stemming from a fixed probability distribution, $p(S|\hat{F}, P, \hat{R})$. Here, we use

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the Differential Evolution Adaptive Metropolis (DREAM) algorithm that was recently introduced by Vrugt et al. (2008, 2009). The DREAM sampling scheme is an efficient MCMC sampler that runs multiple chains simultaneously for global exploration of the search space, and automatically tunes the scale and orientation of the proposal distribution during the evolution to the posterior distribution. This scheme is an adaptation of the Shuffled Complex Evolution Metropolis algorithm (Vrugt et al., 2003) and has the advantage of maintaining detailed balance and ergodicity while showing excellent efficiency on complex, highly nonlinear, and multi-modal target distributions (Vrugt et al., 2009).

In all our calculations reported herein, we assumed that soil temperature and soil moisture are constant and known during the entire incubation experiment. This is a reasonable assumption for controlled laboratory environments. We fixed all model parameters at their standard values (Table 1) and inversely estimated the sizes of the active pools (DPM, RPM, BIO and HUM) at the beginning of the incubation experiment. By definition, the inert pool (IOM) is not decomposed, and hence, observed mineralization rates do not contain any information about the size of this pool. Consequently, its size cannot be estimated from mineralization rate observations. We therefore calculate IOM from the difference between total SOC at the beginning of the experiment and the size of the remaining pools.

2.4 Measurement of microbial biomass carbon

Jenkinson et al. (1992) demonstrated that measured microbial biomass C, C_{BIO} ($g\,C\,kg^{-1}$ soil), as measured using the fumigation-extraction method (Vance et al., 1987) is closely related to simulated C_{BIO} in the ROTHC model. Please note that throughout this paper we use the upper case C to denote measurable C fractions and lower case c to denote model C pools. The basic principle of the fumigation-extraction method is that soil microorganisms die after chloroform fumigation and a part of the microbial constituents is degraded by enzymatic autolysis and transformed into ex-

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tractable components (Joergensen, 1996). Microbial biomass C is calculated as:

$$C_{BIO} = \frac{E_C}{K_{EC}} \tag{7}$$

where E_C (g C kg^{-1} soil) is the organic C extracted from fumigated soil minus that extracted from non-fumigated soil and K_{EC} (dimensionless) is the extractable part of microbial biomass C after fumigation. The K_{EC} value can be obtained from direct or indirect calibration but most of the times a fixed value of 0.45 (Wu et al., 1990) is used. As Joergensen (1996) pointed out, the measurement of E_C is highly precise (having a coefficient of variation CV<5 %), but the estimate of C_{BIO} is less certain owing to the variation of K_{EC} between different soils.

To derive a probability density function of C_{BIO} that can be used as a prior for c_{BIO}, we used the K_{EC} values presented in Joergensen (1996) for arable soils. A normal distribution with mean $\mu=0.42$ and standard deviation $\sigma=0.08$ was shown to fit the reported data well. We used this normal distribution with Eq. 7 to obtain the probability density function of C_{BIO}. This distribution exhibits significant skew to the left, underestimating the actual value. That is, even if the measurement of E_C and the mean of K_{EC} itself are unbiased, the mode of the probability distribution of C_{BIO} does not exactly match its underlying true value. We did not impose a random measurement error on E_C because its magnitude is generally negligible compared to the uncertainty that stems from the natural variability of K_{EC}.

3 Results

3.1 Using non-informative priors

Figure 3 displays posterior marginal probability density functions of the initial pool sizes c_{DPM}, c_{RPM}, c_{BIO}, c_{HUM} and c_{IOM} in the ROTHC model for three different durations of the incubation experiment. In Fig. 3 and all subsequent figures, the x-axes cover the

prior ranges of the estimated pools. Using 300 days of incubation (Fig. 3a) the DPM pool is well defined by calibration against measured mineralization rates. The histogram of DPM follows an approximately normal distribution with relatively small dispersion around its true value. The RPM and BIO pools are also reasonably well iden-
5   tified, yet exhibit significantly more uncertainty with acceptable solutions that extend a larger part of the prior parameter ranges. Unfortunately, measured mineralization rates during the first 300 days of incubation contain insufficient information to warrant the identification of the remaining HUM and IOM pools. Their histograms closely follow a uniform hypercube with ranges that virtually encompass the entire prior distribution.
10   One possible solution to improve the identifiability of the HUM and IOM pools in the ROTHC model, is to increase the duration of incubation. Longer experiments will reveal more insights into SOC dynamics, and hence increase the information content of the observed mineralization data for the various carbon pools. Indeed, the middle and bottom panels demonstrate that the initial pool sizes in the ROTHC model become
15   increasingly better identified when more observations of mineralization rate become available. Intuitively this makes sense, especially for carbon pools with intermediate and slow turnover. After 600 days of incubation (Fig. 3b) the HUM pool is now warranted by calibration against observed mineralization data with a tendency of the probability mass to center around the true value used to generate the synthetic data. Note
20   that there are also some minor improvements for c_{RPM} and c_{BIO}. The best results are found after 900 days of incubation (Fig. 3c). The histograms of the different ROTHC carbon pools are best identified with smallest possible standard deviation around the actual values used to generate the data.

The posterior distribution of the IOM pool (fifth panel in Fig. 3) closely follows the
25   shape of the histogram of HUM. This is not surprising since HUM makes up the largest part of total SOC. Any uncertainty in the estimate of c_{HUM} is therefore propagated into estimates of c_{IOM}. This finding highlights the need for an accurate estimate of c_{HUM}.

To better understand the results shown in Fig. 3 please consider Fig. 4 that presents the correlation structure induced in the posterior probability density distribution of the

ROTHC pools. In general, strong correlation between different pools impairs their iden-
tifiability because a change in one pool can easily be compensated for by a change
in another pool. Figure 4 presents two-dimensional scatter plots of the posterior sam-
ples for selected pairs of ROTHC carbon pools for the 900 days incubation experi-
5 ment. To measure the strength of correlation between individual pools, each panel
also reports the Pearson (linear) correlation coefficient r of the presented data. The
two-dimensional clouds of posterior solutions center around the actual values used
to generate the synthetic mineralization data. Most pools demonstrate considerable
correlation with r values ranging up to –0.97. The only carbon pool that is relatively
10 uncorrelated with the others is DPM, which explains why this particular pool is best
identified in all our artificial incubation experiments. All other pools show strong to very
strong correlation, making it difficult to independently infer their values from measured
mineralization rates. The correlation between the posterior samples of the individual
carbon pools is explained by the pathways of carbon flow within ROTHC (Fig. 1) and
15 the differences between decomposition rate constants (Table 1).

3.2   Using an informative prior for the microbial biomass pool

Our previous results have shown that relatively long incubation times are needed to
appropriately constrain all the carbon pools in the ROTHC model. Such long exper-
iments are not only impractical, but also downplay the utility of inverse modeling for
20 assessing SOC dynamics. This limitation inspires thinking into alternative measure-
ments to reduce uncertainty of the various carbon pools. For instance, lets assume
that soil microbial biomass C was measured separately at the beginning of the incu-
bation experiment using the fumigation-extraction method. Lets also consider that this
measurement is relatively unbiased. Figure 5 shows the results for the same incubation
25 lengths as presented in the previous section, but the prior for BIO now includes explicit
information about microbial carbon. For same lengths of incubation, this informative
prior clearly improves the identifiability of the various carbon pools. Compared to the
results of the non-informative prior depicted in Fig. 3 the histograms are now more tight

with smaller dispersion around their actual values used to generate the synthetic mineralization rate data. These results are not surprising. Information about soil microbial carbon effectively reduces the acceptable ranges of c_{BIO}. This in turn leads to smaller uncertainty in the estimates of the other carbon pools, due to the strong correlations
5 between the posterior samples so evidently apparent in the previous figure. So, the length of incubation can be reduced significantly, when explicit information about soil microbial carbon is available.

When using the incubation-extraction method without calibration, the estimate of C_{BIO} might be biased due to an erroneous estimate of K_{CE}. Here we examine the
10 effect of a biased c_{BIO} prior on the inference of the various ROTHC pools. For that purpose, we assumed that the true K_{CE} was either underestimated or overestimated by one standard deviation. Figure 6 shows the resulting pool size estimates using measured mineralization rate data from 900 days of incubation. Please note that even though the absolute error in the K_{CE} values was identical, the shape of the two c_{BIO}
15 priors and their absolute deviation from the true value are quite different. Similar to the previous results, the biased prior again has a dominating effect on the posterior. However, this time there is some small but distinct deviation of the posterior distribution from the true value used to generate the synthetic mineralization data. Underestimating the actual value of c_{BIO} (Fig. 6a), results in a subsequent overestimation of c_{RPM} and
20 an underestimation of c_{HUM}. This is consistent with the correlation structure between these various pools. Notwithstanding, the estimates are still reasonable, with their true values residing within the 95% confidence intervals of the respective posterior distributions. When the actual value of c_{BIO} is overestimated (Fig. 6b) this bias is easier mitigated, with closer estimates of the remaining pools.

25 **4 Discussion**

The results presented in this paper demonstrate that it is generally feasible to estimate the initial sizes of all active pools in the ROTHC model from observed mineralization

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rates during incubation. The currently available technique for measuring mineralization rates in an automated manner is sufficiently accurate to warrant the simultaneous identification of all carbon pools. The Bayesian approach has proven especially useful in this context.

Independent measurements of microbial biomass further improves the estimation of the various carbon pools. A comparison of Fig. 3 (non-informative prior) with Fig. 5 (informative prior for c_{BIO}) reveals that informative priors allow for much shorter durations of incubation. However, we highly recommend making use of direct calibration such as in situ labeling of microorganisms (Bremer and van Kessel, 1990; Dictor et al., 1998) to assure that the estimate of C_{HUM} is unbiased. This is important because a bias in the c_{BIO} prior is not necessarily fully balanced for by the information contained in the observed mineralization data. This bias may also lead to errors in the estimates for c_{RPM}, c_{HUM}, and consequently c_{IOM}. Moreover, Dictor et al. (1998) showed how to calculate the standard deviation of the sample distribution of K_{CE} derived from replicate in situ labeling measurements. This information can directly be used to formulate an informative prior which, based on the data given in Dictor et al. (1998), is much more accurate than the prior used in this study. Given the importance of c_{BIO} in our multi-compartment SOC modeling, it would be desirable to further improve the accuracy of this measurement. Furthermore, a more reliable estimate of c_{BIO} would enable us to judge whether measured microbial biomass is related to its ROTHC modeled counterpart. This is of particular relevance, because the results of Jenkinson et al. (1992) have not yet been verified.

It is particularly difficult to make a general statement about the appropriate duration of an incubation experiment. This not only depends on the quality of the measurement equipment, but also on the desired level of accuracy in the estimated carbon pools. The smaller the measurement error, the smaller the uncertainty in the estimated pool sizes. Yet, the high correlation between individual carbon pools still requires a minimal incubation length of at least several hundred days. This is especially true for intermediate and slow pools. Such duration seems impractical for most applications.

Fortunately, explicit use of an informative prior for the microbial biomass pool substantially reduces the incubation time required to obtain statistically sound estimates of the various carbon pools. For most practical applications, we therefore recommend using such informative prior.

5   Given the significant duration of incubation we argue that modeling and data collection should go hand in hand. There is no need to continue data collection if measurements are redundant or do not further reduce uncertainty in the estimands. A sequential Bayesian filter that updates the posterior distribution of the various carbon pools every time new mineralization data becoming available would be especially useful

10 within the current context as it provides important diagnostic information to help judge when to stop the experiment. This would not only speed-up the experimental analysis, but also provide important cost savings. The Bayesian approach utilized herein could also prove useful to independently test the fractionation methods proposed by Skjemstad et al. (2004) and Zimmermann et al. (2007) by comparison of measured fractions

15 with estimated and predicted pool sizes. Future work should also focus on evaluate ROTHC against a time series of observed microbial biomass C. This will help establish whether ROTHC can describe the decline in microbial biomass which is commonly observed during long-term incubation experiments (e.g. Nicolardot et al., 1994; Follett et al., 2007). Finally, the modeled decomposable and resistant plant material pools

20 could be compared to measured light fraction C.

5   Conclusions

The results presented in this paper highlight that it is generally feasible to estimate the initial sizes of all active pools in the ROTHC model from data collected during incubation experiments. The current available techniques to measure mineralization rates are

25 sufficiently accurate to provide all necessary information. The use of prior information on the size of the microbial biomass pool has the potential to substantially reduce the incubation time needed to obtain accurate estimates of the various pool sizes. This

is especially useful for assessing pools with slow and intermediate carbon turnover. Altogether, our results demonstrate that Bayesian inverse modeling provides important insights into the information content of mineralization rate data, and is especially helpful in the testing of conceptual multi-compartment SOM models and fractionation methods.

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Table 1. Pool sizes and parameter settings in the ROTHC model used to generate the synthetic time series of mineralization rate measurements. Abbreviations stand for decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO), humified organic matter (HUM), and inert organic matter (IOM).

symbol	description	value	unit
c_{DPM}	initial pool size DPM	0.2	$g\,C\,kg^{-1}$ soil
c_{RPM}	initial pool size RPM	3.7	$g\,C\,kg^{-1}$ soil
c_{BIO}	initial pool size BIO	0.5	$g\,C\,kg^{-1}$ soil
c_{HUM}	initial pool size HUM	20.4	$g\,C\,kg^{-1}$ soil
c_{IOM}	pool size IOM	3.8	$g\,C\,kg^{-1}$ soil
k_{DPM}	decomposition rate constant DPM	10.00	$year^{-1}$
k_{RPM}	decomposition rate constant RPM	0.30	$year^{-1}$
k_{BIO}	decomposition rate constant BIO	0.66	$year^{-1}$
k_{HUM}	decomposition rate constant HUM	0.02	$year^{-1}$
$f_1(T = 20\,°C)$	rate modifier for temperature	2.83	dimensionless
$f_2(\theta = optimal)$	rate modifier for soil moisture	1.00	dimensionless
$f_3(\gamma = bare)$	rate modifier for vegetation cover	1.00	dimensionless
$p_2(clay = 23\,\%)$	partitioning coefficient	0.78	dimensionless
p_3	partitioning coefficient	0.46	dimensionless

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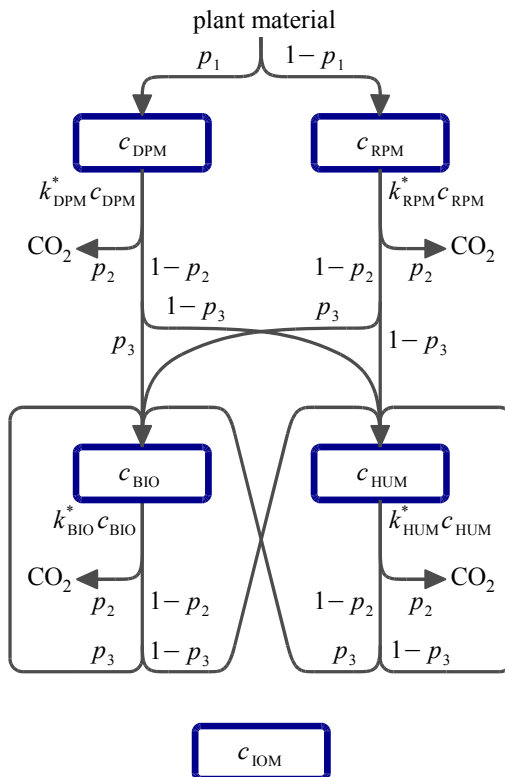
Fig. 1. Structure of the ROTHC model. The model has four active pools: decomposable plant material (c_{DPM}), resistant plant material (c_{RPM}), microbial biomass (c_{BIO}) and humified organic matter (c_{HUM}). The inert organic matter pool (c_{IOM}) is assumed to be passive. Three partitioning coefficients (p_1, p_2 and p_3) govern the flow of carbon. See text for more information.

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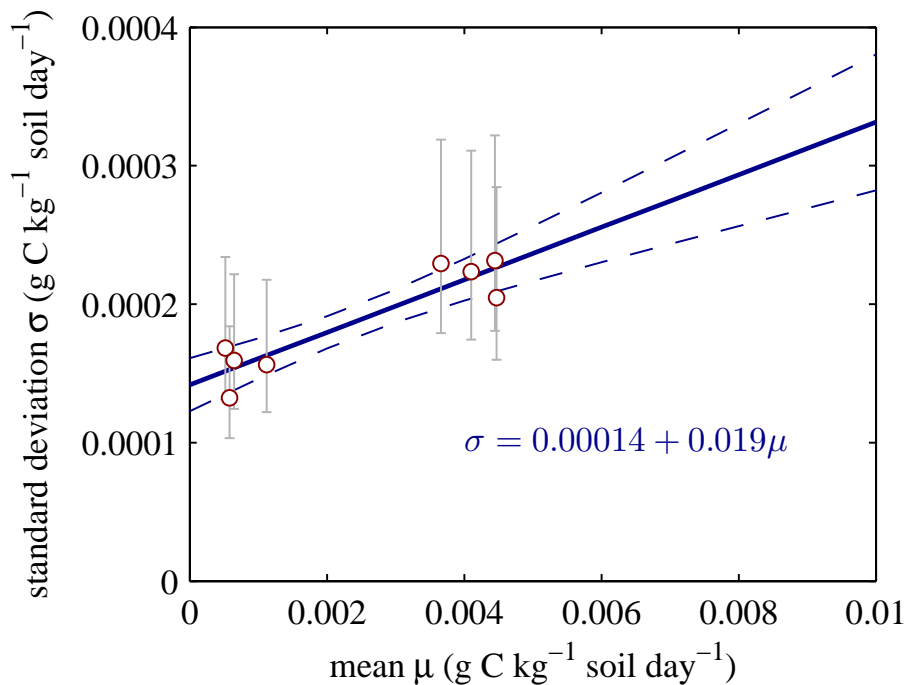
Fig. 2. Precision of mineralization rate measurements using an automated respirometer. The circles show the measurements, error bars mark the 95% confidence intervals. The solid line represents the fitted error model, whereas the dashed lines mark the 95% confidence intervals.

$$\sigma = 0.00014 + 0.019\mu$$
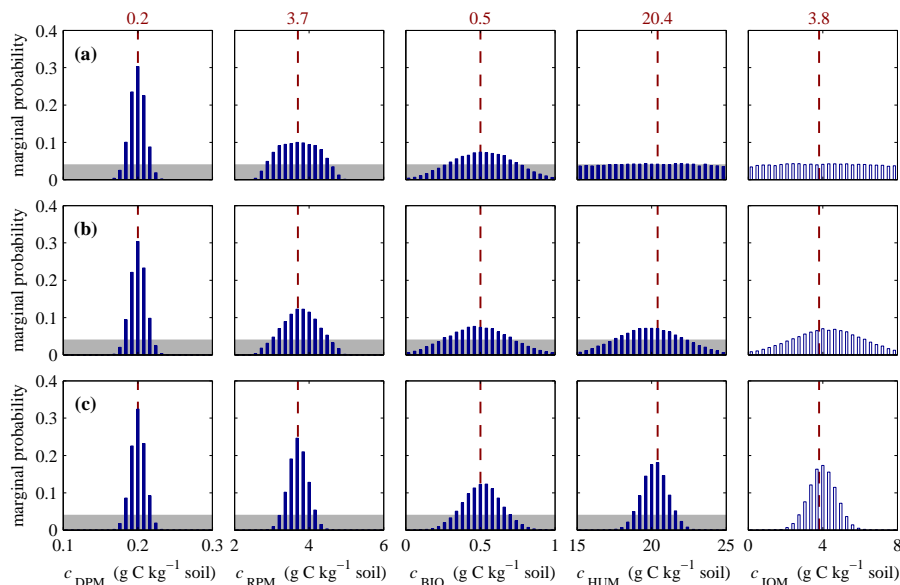
Fig. 3. Posterior marginal probability density distributions of initial pool sizes using a non-informative prior: **(a)** 300 days of incubation, **(b)** 600 days of incubation, and **(c)** 900 days of incubation. Only the size of the four active pools (DPM, RPM, BIO and HUM) were estimated. The size of the inert pool (IOM) was calculated by difference from total SOC. The gray area shows the prior probability distribution. The dashed lines mark the true values used to generate the synthetic data.
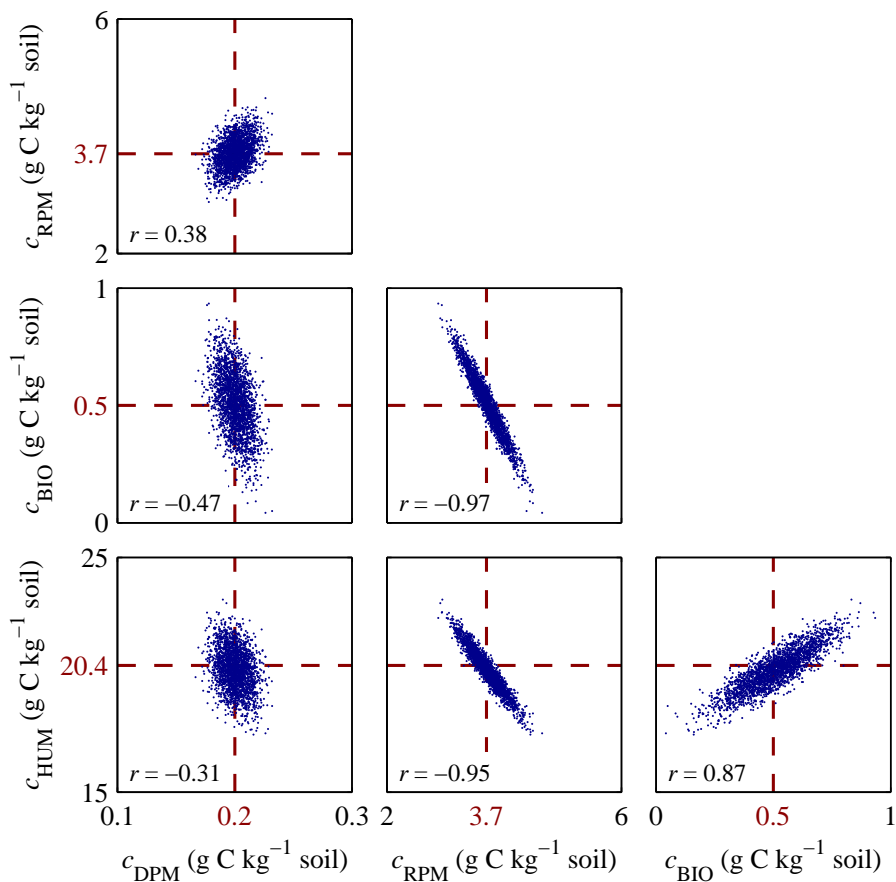
Fig. 4. Scatter plots of posterior samples for selected pairs of the active carbon pools. Results correspond to 900 days of incubation. Dashed lines mark the true values, and Pearson coefficients (r) illustrate strength of correlation between individual carbon pools.
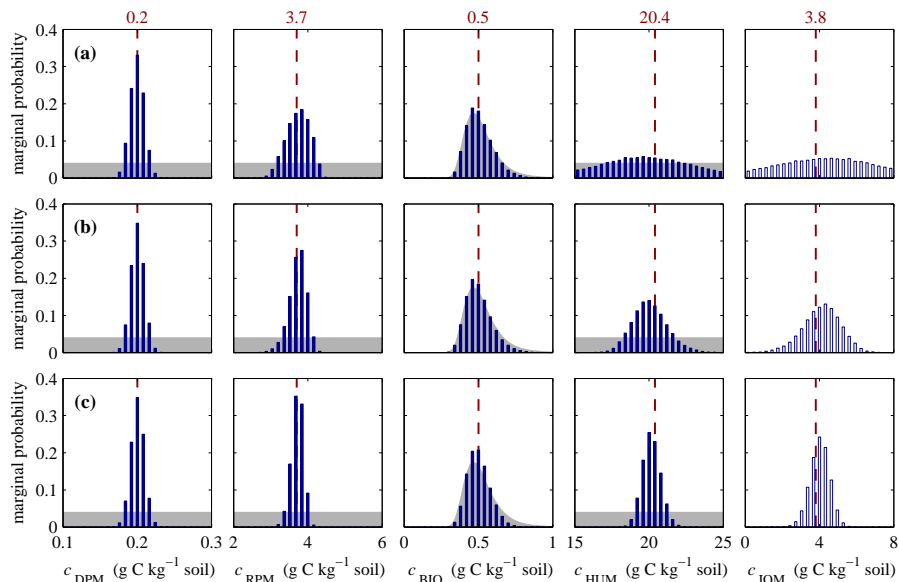
Fig. 5. Posterior marginal probability density distributions of initial pool sizes using an unbiased informative prior for the microbial biomass pool: **(a)** 300 days of incubation, **(b)** 600 days of incubation, and **(c)** 900 days of incubation. We only consider the four active ROTHC pools (DPM, RPM, BIO and HUM). The size of the inert pool (IOM) was calculated by difference from total SOC. The gray area shows the prior probability distribution. The dashed lines mark the true values used to generate the synthetic data.
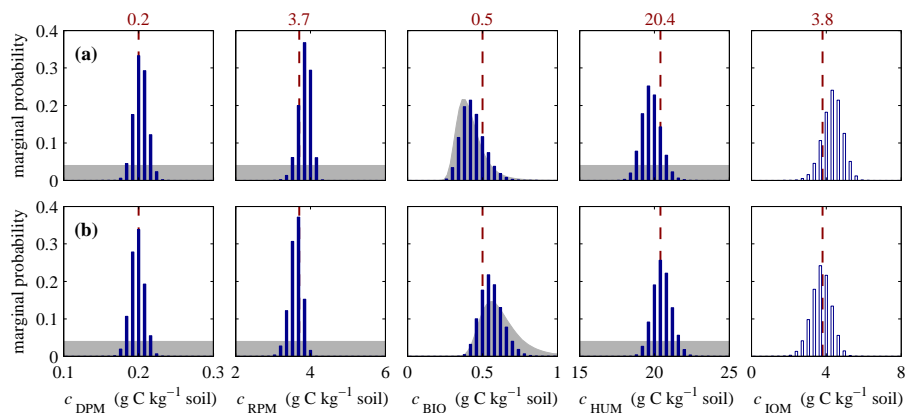
Fig. 6. Posterior marginal probability density distributions of initial pool sizes using a biased informative prior for the microbial biomass pool: **(a)** underestimation, **(b)** overestimation of the true value. We used 900 days of incubation. Only the four active ROTHC pools are depicted (DPM, RPM, BIO and HUM). The size of the inert pool (IOM) was calculated by difference from total SOC. The gray area shows the prior probability distribution. The dashed lines mark the true values.

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