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Optimizing duration of incubation experiments for understanding soil carbon decomposition

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ABSTRACT

Laboratory incubation is a commonly used method to measure the decomposition of soil organic carbon (SOC). While incubation experiments are conducted across a wide range of durations that may vary from hours to years, no method is available to determine an optimal duration of the incubation experiment so that SOC decomposition can be best understood. Here we presented a novel approach to determine the optimal duration called OPtimal Incubation Duration (OPID). The OPID approach quantifies information gained from an ongoing incubation experiment and determines the time point when SOC decomposition rates can be well quantified. Statistically, the OPID approach is based on a progressive data assimilation algorithm that iteratively assimilates data from an ongoing incubation experiment into a three-pool first-order SOC decomposition model. Using a published incubation data set under different temperatures as a case study, we first generated synthetic daily data, and then fed the data into the three-pool model iteratively to observe the changes of model performance. We found that the accuracy of model projections increased with incubation period and exhibited a trade-off between initial model performance and the time towards accurate projection among different temperatures of incubation. The optimal incubation duration was 347, 212, and 126 days under incubation temperatures of 15 °C, 25 °C and 35 °C, respectively. Comparing the parameters with which from the synthetic daily data, if the incubation period was shorter than the optimal durations, then the decomposition rate of the fast-turnover pool was underestimated and those of the slow pools were overestimated. Sensitivity analysis indicated that optimal incubation duration was negatively correlated with proportion of slow-turnover carbon pools, turnover rates, and initial carbon content, respectively. Our study suggested that long-term incubation experiments are necessary for capturing the dynamics of slow-turnover carbon pools. However, the additional data may not be helpful for model performance if the incubation duration is longer than the optimum. Our study provides a tool for soil scientists to design more effective incubation experiments.

DA: data assimilation; PDA: progressive data assimilation; Cum CO_2: cumulative CO_2 emission from soil; opt: optimal duration;

1. Introduction

Globally, soils store ~3000 Pg of organic carbon (C) (Andriamananjara et al., 2017; Giardina et al., 2014; Jobbágy and Jackson, 2000; Tarnocai et al., 2009), four times more C than the atmosphere, and six times more than vegetation (German and Allison, 2011; Goulden et al., 2001). Soil releases ~100 Pg C to the atmosphere as CO_2 each year (Bondlamberty and Thomson, 2010; Karhu et al., 2014). An important part of soil CO_2 efflux is the product of SOC decomposition via microbial respiration. The predicted future global warming may have important

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consequences for the emission of CO_2 from soils as a positive feedback to the global C cycle (Cox et al., 2000; Knorr et al., 2005; Rey et al., 2010). In addition to the importance of SOC in the global terrestrial carbon cycle as the largest terrestrial carbon pool and as the source of one of the largest terrestrial carbon fluxes, soil organic matter turnover is a key factor in soil fertility and nutrient replenishment. Therefore, a better understanding of the decomposition of soil organic carbon is important (Ahrens et al., 2014).

Laboratory incubations of soils under controlled environmental conditions have widely been used to measure C mineralization and investigate the environmental factors such as temperature and moisture controlling the decay of different pools (Dalias et al., 2001; Rey and Jarvis, 2006). The method allows control of the environmental variables and can compare the mineralization rates of soil samples from different locations under standardized conditions. Normally, the labile proportion of C pools could be decomposed rapidly, but it takes a long time for slow turnover C pools to be decomposed (Zou et al., 2005). In the literature, incubation experiments have been conducted with a wide range of durations that vary from hours to years (Jian et al., 2020). The majority of incubation experiments lasted less than one year (Fig. S1), of which 45.87 % of the studies were less than 60 days. When feeding incubation data to SOC decomposition models, different sections of the data contain uneven information for different soil pools. Due to the fast turnover rates of active pools, most of the CO_2 released by SOC comes from the fast-decomposing part at the beginning of incubation, so the first few days of incubation data are obviously generated more from fast-decomposing SOC. Soil incubation studies that last longer than 100 days may contain more contributions from slow-decomposing C-pools (Lützow and Kögel-Knabner, 2009). Therefore, model parameters estimated from short- and long-term incubation dataset are quite different (Hararuk and Luo, 2014; Li et al., 2019). The inconsistency in incubation period across studies makes it difficult to compare SOC decomposition rates.

Previous studies suggested that long-term incubation experiments are necessary for estimating carbon pools with slow turnover rates (Jian et al., 2020), but no studies have quantified how long of an incubation period is necessary or if the incubation period should be as long as possible. Researchers usually do not describe the details of how to determine the incubation period in their study. It is known that a decline in the rate of decomposition is usually observed with the proceeding of incubation (Fang et al., 2005; Xu et al., 2010). They usually terminate the incubation experiment empirically, or when they think the rate of mineralization is stabilized. However, there exist different judgments of stability, and lead to large uncertainty in determining incubation period.

Many process-based models have been developed to simulate the dynamics of SOC (Jenkinson et al., 1987; Katterer et al., 1998; Liang et al., 2015b; Luo et al., 2001). Most prevalent models use first-order kinetics, i.e. dividing SOC into multiple pools with cascading decomposition rates modified by different environmental attributes such as climate and soil properties (Stefano and Amilcare, 2009). Therefore, decomposition rates of different C pools could be estimated by fitting the data from incubation experiments to the model. Although the model structure is simple, large uncertainties exist in the estimation of parameters (Toddbrown et al., 2014; Verstraeten et al., 2008; Yan et al., 2014).

Data assimilation (DA) is an effective approach to reduce the uncertainties, by integrating observations of C efflux from incubation experiments. (Ahrens et al., 2014; Li et al., 2013). The fundamental notion of DA is the capability of feeding into a model iteratively and updating posterior parameters based on prior information (Schadel et al., 2013; Wieder et al., 2015; Yan et al., 2014). DA improves model parameters and the forecasts using information contained in observational data to obtain the posterior probability distributions of targeted parameters. Data assimilation can improve ecological forecasting by providing a probabilistic analysis to evaluate sampling strategies for future experiments and observations that will enable improvements to models and forecasts (Hood et al., 2007; Luo et al., 2011). Recently, the approach has been used to estimate soil carbon dynamics and responses of SOC to environmental factors such as temperature and moisture (Luo et al., 2020). Cumulative CO_2 emission data of an incubation experiment come from decomposition of different components of SOC varying from labile to recalcitrant organic carbon. By feeding the data into a SOC decomposition model, one can inversely estimate the turnover rates of different SOC components.

To explore the optimal incubation period that could be used to accurately estimate decomposition rates of different C pools, we first need to investigate how model projection is influenced by the length of the incubation period. Here, we developed a progressive data assimilation algorithm that feeds reliable incubation data iteratively to constrain a first-order three-pool SOC decomposition model. Then, we used an observing system simulation experiment to address three specific questions: (1) is there an optimal incubation duration where additional experimental data do not significantly improve model performance; (2) how do temperatures influence the projection accuracy under different lengths of incubation data; and (3) how do the optimal length of incubation period changes with model parameters?

2. Materials and methods

The OPID approach used a three-pool SOC decomposition model and the progressive data assimilation algorithm to get the optimal incubation duration of incubation experiments. To test the robustness of the algorithm, we first estimated parameters of a three-pool SOC decomposition model using a case study of an incubation experiment. Then, synthetic daily data were generated from the estimated parameters. The synthetic daily data were treated as ‘observations’, which normalized data frequency in daily steps and eliminated sampling errors. This is widely known as an observing system simulation experiment (OSSE) in numerical weather prediction, which can be used to investigate the behavior of data assimilation systems (Arnold and Dey, 1986; Zeng et al., 2020). By feeding the synthetic data into the model continually, we can determine whether and when the constrained parameters could match true parameters, and how the uncertainty of forecasting changes. The optimal incubation duration could be reached when parameters are accurately estimated and the forecasted cumulative CO_2 emissions match ‘observations’. At the end, we tested the algorithm using real data from the case study of an incubation experiment.

The calculation of the optimal incubation duration was as follows: (1) derive maximum likelihood estimates of model parameters (Table 1) from the incubation data of Haddix et al. (2011) as a case study; (2) use the parameters to generate a time series of 600 days daily incubation data, treated as ‘observations’, named synthetic data here after; (3) use the first n_0 days of the synthetic data, $n_0 = 10$ in this paper, to constrain the mineralization rates (k_i) by the Metropolis-Hastings (M−H) algorithm; (4) update parameters k_i when adding new data points of the synthetic data; (5) update the prior parameter distribution using outputs from the posterior distribution, and repeat until all synthetic data is used; (6) use a *t*-test to get the difference between model predictions and the synthetic data for each data assimilation; and (7) calculate the optimal incubation duration by using logic regression of the binary outputs from the *t*-test. The R script can be found in the online supplemental materials.

2.1. Source of soil incubation data

Original soil incubation data used in this study were extracted from Haddix et al. (2011), which has been used for fitting multiple SOC decomposition models (Li et al., 2013; Liang et al., 2015a; Xu et al., 2010). The soil was obtained from cultivated land in Indian Head, Saskatchewan, Canada (50.533°N, 103.517°W). The mean temperature was 2 °C and precipitation was 421 mm. Information about soil sampling and incubation detail was described in Haddix et al. (2011). Briefly, the soil

Table 1
The range and value of parameters used for data assimilation.

Parameter	Description	15C		25C		35C	
		min	max	min	max	min	max
k_1	Decomposition rate of active pool ($mg \bullet g^{-1} Cd^{-1}$)	3.25E-04	7.32E-02	6.81E-04	1.53E-01	1.40E-03	3.17E-01
k_2	Decomposition rate of slow pool ($mg \bullet g^{-1} Cd^{-1}$)	7.22E-06	1.60E-03	1.45E-05	3.30E-03	3.83E-05	8.60E-03
k_3	Decomposition rate of passive pool ($mg \bullet g^{-1} Cd^{-1}$)	1.41E-06	3.17E-04	2.63E-06	5.91E-04	3.62E-06	8.14E-04

Parameter	Description	value
f_1	fraction of active pool (%)	4.65
f_2	fraction of slow pool (%)	14.53
f_3	fraction of passive pool (%)	80.82
C_{tot}	initial carbon content (g/kg)	22.9

samples were incubated at 15, 25, and 35 °C, respectively, for 588 days (number of laboratory replicates = 3). In the first two weeks, CO_2 emission rates were measured daily, then weekly for the next two weeks, and every-four weeks for the last 80 weeks. Overall, there were 36 samples over the 588-day incubation. Data at all the 15, 25 and 35 °C were used to estimate parameters of the three-pool SOC decomposition model.

2.2. Model description

We used a classic three-pool first-order SOC decomposition model (Katterer et al., 1998; Liang et al., 2015a). The model contains three SOC fractions representing different physicochemical properties with different turnover time. An active pool consists of living microorganisms and microbial products as well as soil organic matter with a short turnover time (1–5 yr); a slow pool is physically protected and/or chemically recalcitrant, with more biological resistance to decomposition and an intermediate turnover time (20–40 yr); and a passive pool is stabilized by mineral protection, with the longest turnover time (200–1500 yr) (Morra and Dick, 1989). The process of SOC mineralization can be described in the function below.

$$\frac{dC_i}{dt} = k_i C_i \tag{1}$$

$$C_i(t=0) = f_i C_{tot}$$

$$\sum_{i=1}^{n} f_i = 1$$

where C_i is carbon pool size of fraction i, with C_1, C_2, and C_3 represents active, slow, and passive pools, respectively. f_i and k_i are the initial fraction and mineralization rate of the i^{th} pool. The sum of f_i is 1. The change in C pool size for fraction i was modeled by a first order differential equation with C-pool i decaying at a temperature-dependent rate k_i over time (t) multiplied by the dynamic C pool size. C_{tot} is the total initial C of the three pools, which is 22.9 g/kg soil when t = 0, based on the curve fitting of Haddix et al. (2011).

2.3. Progressive data assimilation (PDA)

We used a probabilistic inversion approach based on Bayesian framework to drive posterior probability density function of parameters k_i in this paper, as in (Xu et al., 2016).

$$P(\theta|Z) \propto P(Z|\theta) P(\theta) \tag{2}$$

Where posterior probability density function $P(\theta|Z)$ of the model parameters (θ) can be obtained from prior knowledge of parameters represented by a prior probability distribution $P(\theta)$ and information in the soil incubation data represented by the likelihood function $P(Z|\theta)$. The prior probability density function was specified as the uniform distributions over a range of a specific parameter (Liang et al., 2015a; Xu et al., 2016). Ranges in this paper are shown in Table 1 based on Liang et al (2015). The likelihood function $P(Z|\theta)$ was calculated under the assumption that errors between observed values and modeled values were independently distributed according to the equation:

$$P(Z|\theta) \propto exp\left\{ -\frac{1}{2\sigma^2} \sum_{t \in obs(Z_i)} [Z_i(t) - X_i(t)]^2 \right\} \tag{3}$$

where Z and X are the observed and modeled cumulative CO_2 emission values, respectively, and σ is the standard deviation of measurements.

The probabilistic inversion is performed using the M−H algorithm, which is a Markov Chain Monte Carlo (MCMC) technique (Liang et al., 2015a), for constructing the posterior PDFs of parameters. Briefly, the M−H algorithm repeats the proposing step and moving step. In the proposing step, a new θ^{new} is generated based on the previously accepted point θ^{old} with a proposal distribution $P\left(\theta^{new}|\theta^{old}\right)$:

$$\theta^{new} = \theta^{old} + \frac{r(\theta_{max} - \theta_{min})}{D} \tag{4}$$

where θ_{max} and θ_{min} are the maximum and minimum values in the prior range of the given parameter, r is a random variable between −0.5 and 0.5 with a uniform distribution, and D is used to control the proposing step size and was currently set to 20. In the moving step, the new point θ is tested according to the Metropolis criterion to examine if it should be accepted or rejected. Because the initial accepted samples are in the burn-in period (Xu et al., 2006), the first half of accepted samples were discarded and only the remaining were used to generate posterior PDFs. The M−H algorithm was formally run 500,000 times for each lab incubation data.

In this paper, daily synthetic data adding one by one fed in progressive data assimilation after standardized. We recorded the posterior distribution of parameters and projected SOC dynamics after each of the data assimilation. Ideally, the projected SOC dynamics would match the synthetic data; the constrained parameters would equal the parameters we used to generate synthetic data. However, using part of the data could result in bias in parameter estimations and projected SOC dynamics. We calculated the root-mean-square error (RMSE) between synthetic data and the model simulations after each of the data assimilation.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (mod_i - obs_i)^2}{n}} \tag{5}$$

where mod_i is the mean value model predicted for each day, obs_i is the synthetic data of cumulative CO_2, and n is 600 as the number of days.

2.4. Optimal incubation duration and the sensitivity analysis

We assumed that the optimal length of an incubation experiment could be reached when the forecasted cumulative CO_2 emission matched the synthetic data, given the first-order decay model. Model prediction from each data assimilation with part of the synthetic data should be compared with the whole data set to determine whether model prediction could match synthetic data. First, we applied a *t*-test to find the difference between model predictions and the synthetic data at day 600 for each single data assimilation. We produced a series of binary values (1, 0), where 1 indicated a significant difference and 0 was non-significant, for different lengths of incubation data. To determine the optimal incubation duration, we performed generalized linear regression using the 'logit' link function on the binary data. The turning point, where the second derivative of the fitted line equals to 0, was considered to be the optimal duration.

Sensitivity analysis was performed to assess how the optimal duration would be influenced by the parameters (f_1, f_2, k_1, k_2, k_3) and initial soil carbon content (C_{tot}), representing different soil properties. We used a Latin hypercube sampling (LHS) algorithm (Mckay et al., 1979) to produce 5,000 sets of parameters values. The LHS algorithm allows an unbiased estimate of the average model output, which requires fewer samples than simple random sampling. We then calculated the parameter sensitivity index using the partial rank correlation coefficient (PRCC), which performs a partial correlation between specific parameter and model outputs based on rank-transformed data. PRCC is a robust sensitivity measure for nonlinear but monotonic relationships between parameters and model outputs (Marino et al., 2009; Moore et al., 2015). Finally, generalized linear regression was performed to explore the relationships between optimal duration and the parameters containing information of decay rates, pool composition, and SOC content.

3. Results

3.1. Constrained parameters change with incubation period

We first investigated when the constrained parameters from progressive data assimilation could match the given parameters from the synthetic data. We found that most estimated parameters were well constrained. However, the constrained values were biased if incubation periods were not long enough (Fig. 1). The mineralization rate of active pool (k_1) was overestimated at the very beginning of the incubation experiment, and then was underestimated until 375 days later. The mineralization rate of slow pool (k_2) and passive pool (k_3) were overestimated for short periods of incubation. With the incubation period increases, the estimated parameters approach true values. Although the biases to true parameter values were larger at higher temperatures, the time to approach true values seemed to be shorter. For example, at the incubation temperature of 15 °C, the estimated parameters matched true

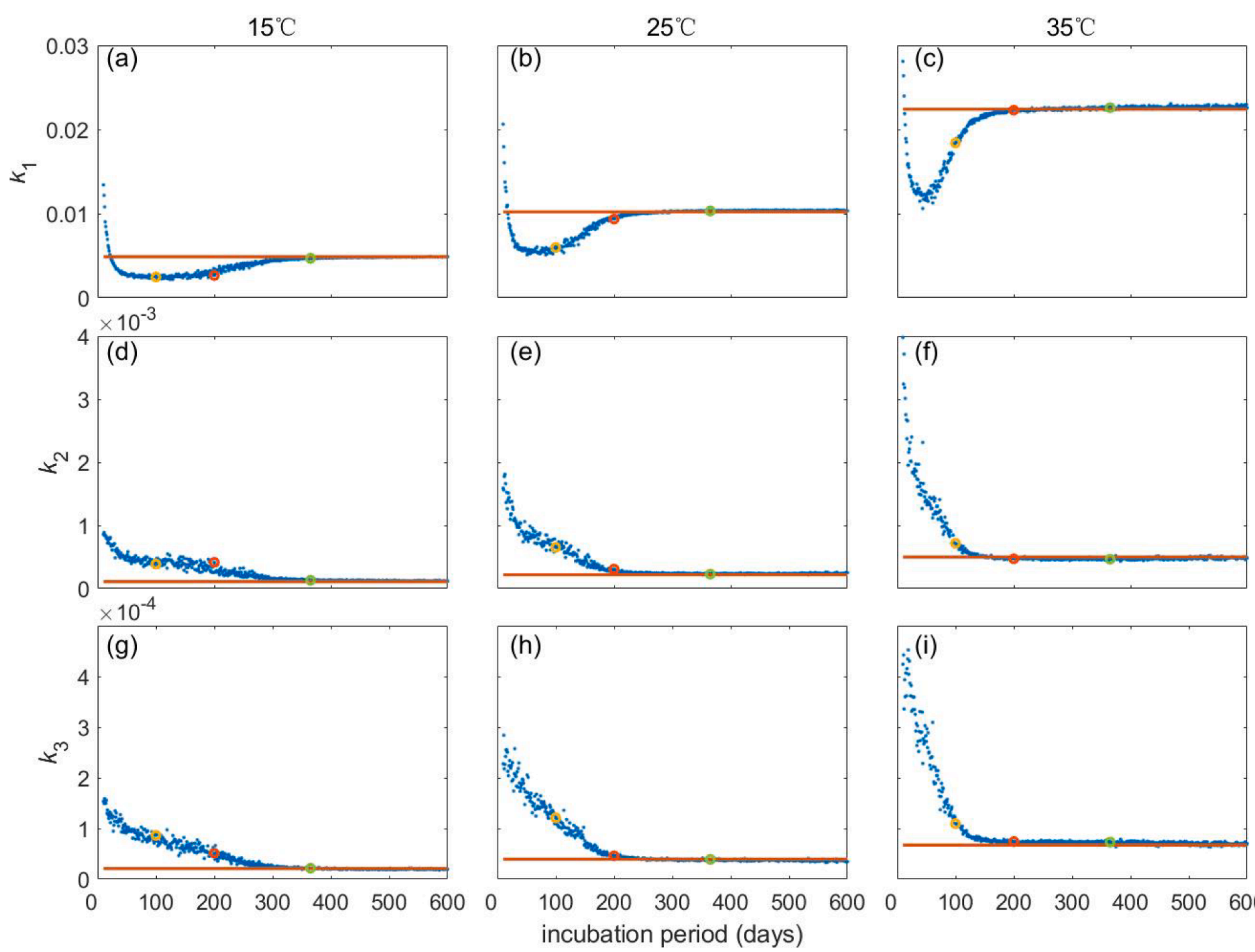

Fig. 1. Constrained decomposition rates (k_1, k_2, k_3) under different incubation temperatures (15 °C 25 °C, and 35 °C) and different incubation periods. Constrained decomposition rates are derived from the Progressive Data Assimilation (PDA) and the synthetic CO_2 emission data are used as observations of the PDA. Red lines are the given parameter values which generated the synthetic CO_2, the blue points corresponding to the mean values of posterior parameters distribution for each day of PDA. The three circles in yellow, red and green are parameter values picked at day 100, 200, and 365 for Fig. 2.

values around one year of incubation, whereas at 35 °C, parameters matched true values at roughly half of a year.

3.2. Performance of model predictions

The performance of model predictions improved with increased incubation period (Fig. 2). The prediction of soil organic carbon mineralization was overestimated when short-term incubation data were used, e.g., 10 days of incubation under 25 °C (Fig. 2a). As the incubation experiment lasted longer, the model's predictions gradually approached the generated synthetic data. The uncertainty of model predictions was also reduced with increasing incubation period. The model predictions under incubation temperature of 15 °C and 35 °C were similar to that of 25 °C (Fig. S2, Fig. S3). It was further confirmed that the overestimated cumulative CO_2 emission mainly resulted from an overestimated contribution of slow and passive pools (Fig. S4).

As expected, RMSE decreased with the incubation period (Fig. 3). After a certain incubation period, the predictions match data well and the RMSE was close to 0. When short-term incubation data were used, say less than 60 days, the RMSE was larger under higher incubation temperature than lower ones (Fig. 3a). However, the RMSE dropped faster under higher incubation temperature when additional data were fed into the model. When using the real experimental data for the progressive data assimilation, we found similar patterns in changes of model performance with increasing incubation period (Fig. 3b).

3.3. Optimal duration and sensitivity analysis

There was an optimal length of incubation period below which model projections differed significantly from the 'observation' at day 600. The optimal duration was shorter under higher incubation temperature. For example, the optimal duration of incubation experiment was 347, 212, and 126 days in 15, 25, and 35 °C, respectively, for the parameter settings of our study (Fig. 4).

Sensitivity analysis showed that the optimal duration was related to initial soil carbon content (C_{tot}), decomposition rates, and the relative fraction of different carbon pools (Fig. 5). A shorter length of incubation period was needed for soils with higher C_{tot}. The optimal duration also decreased with the decomposition rates, especially for the fast turnover pools. Soil with a higher fraction of active pool needed a longer incubation period to get the optimal duration. Consistent with the PRCC, when changing each parameter separately, optimal duration increased with f_1 linearly, but decreased with other parameters (Fig. S5).

4. Discussion

4.1. Length of incubation duration

Soil incubation is a useful method to measure the decomposition rate of SOC. However, almost all the incubation experiments of SOC decomposition do not justify how they determine the duration of their experiments. Experiments longer than 200 days are considered a long-

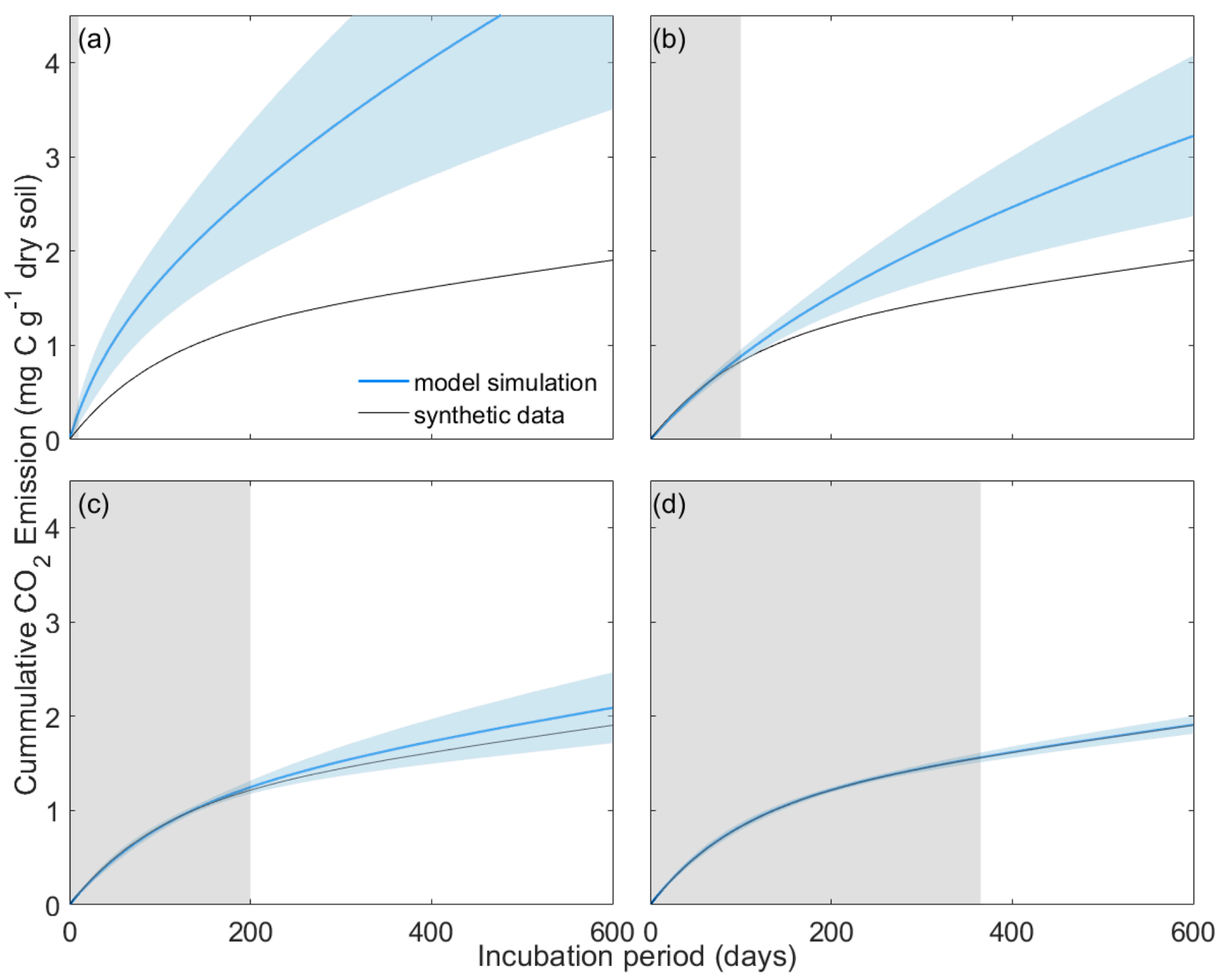

Fig. 2. The observed and predicted cumulative CO_2 emission under 25 °C when different incubation data are fed into the PDA model. Incubation data of (a) 10, (b) 100, (c) 200, and (d) 365 days. The gray shaded area denotes the data used in the PDA model. The blue lines show the mean predicted cumulative CO_2 emission using model simulation, and the light-blue areas represent the mean ± standard deviation ranges of the model prediction.

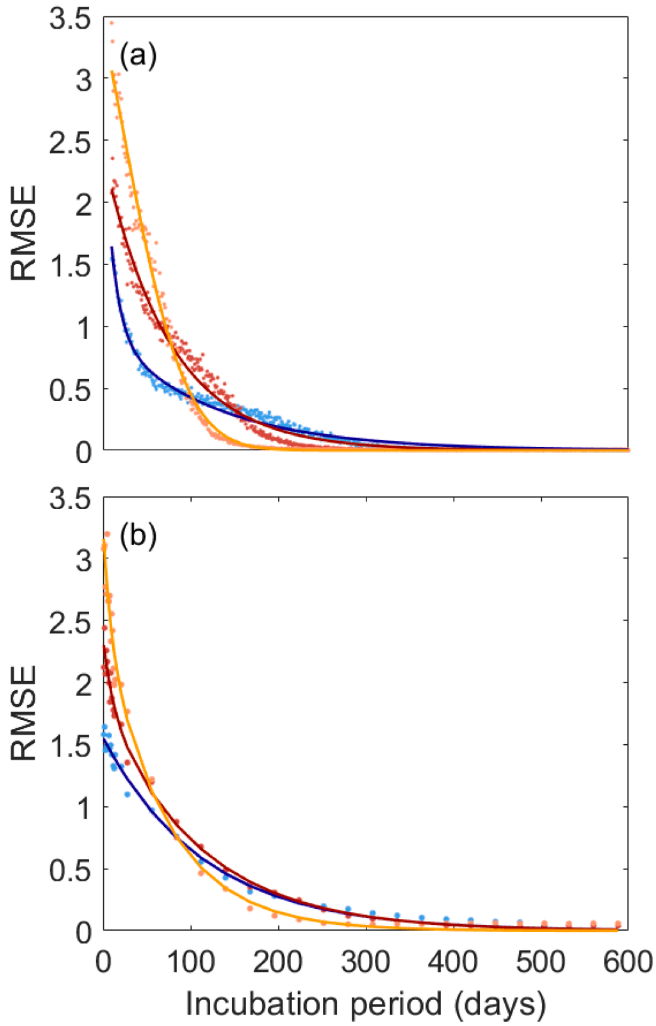

Fig. 3. RMSE between model outputs and incubation data under different incubation temperatures. (a) Synthetic data and (b) real data. Scatters and lines in color represent the RMSE value and fitting lines in 15 °C (blue), 25 °C (red), and 35 °C (orange).

term incubation experiment (Rey and Jarvis, 2006). Despite the general agreement that long-term incubation is needed to estimate the mineralization rate of the recalcitrant fractions of soil C, no studies can tell how long of an incubation period is sufficient. Our study indicated that most short-term studies might not be able to capture the dynamics of slow-turnover carbon pools so that SOC decomposition would not be reliably quantified. Using the OPID approach we developed, we identified the optimal duration of incubation length, i.e., ~ 347, 212, and 126 days under temperatures of 15, 25, and 35 °C, respectively, given our parameter settings. Temperature is one key variable that often determines the length of an incubation experiment. Our results were consistent with general knowledge that temperature is a factor that has the greatest influence on soil organic carbon mineralization (Shi et al., 2020).

Most of the short-term incubation experiments were aimed at obtaining the soil mineralization rate of labile carbon (Schädel et al., 2020; Wang et al., 2020; Xu et al., 2010), or to explore certain treatment effects (e.g. nitrogen additions and land use changes) on soil organic carbon mineralization (Liu et al., 2019; Wang et al., 2019). However, if the purpose of the study was to learn the long-term process of soil mineralization, short-term incubation data are not enough to provide sufficient information on decomposition rates of slow turnover pools. Parameters estimated from short-term datasets are usually higher than those from long-term datasets (Li et al., 2019). Zou et al. (2005) used a fumigation-incubation procedure to obtain pool sizes and potential turnover rates of different fractions of soil organic carbon through measuring microbial biomass. They found that a period of less than three months can get enough mineralization information of labile organic carbon. However, it is difficult to obtain the characteristics of a stable carbon pool within such a short period. Therefore, most incubation experiments reported in literature were less than three months (59 %) (Fig. S1), and thus could not have captured mineralization information of stable carbon pools. A study by Schadel et al. (2013) found that data from a long-term incubation of 385 days was not able to well constrain parameters of the passive pool, which was longer than our evaluation. This difference was probably due to a much lower fraction of the passive pool (only 22 %) in their study than the data we used from Haddix et al. (2011).

Uncertainty in parameter estimation, especially SOC decomposition rates, is one of the main sources of uncertainties in soil C dynamics prediction (Jiang et al., 2018; Luo et al., 2016). Using the three-pool model, we found that the decomposition rates of slow-turnover and passive-turnover pools were overestimated, while the fast-turnover pool was underestimated when short-term data were fed into the model. These discrepancies were probably because information from the fast-

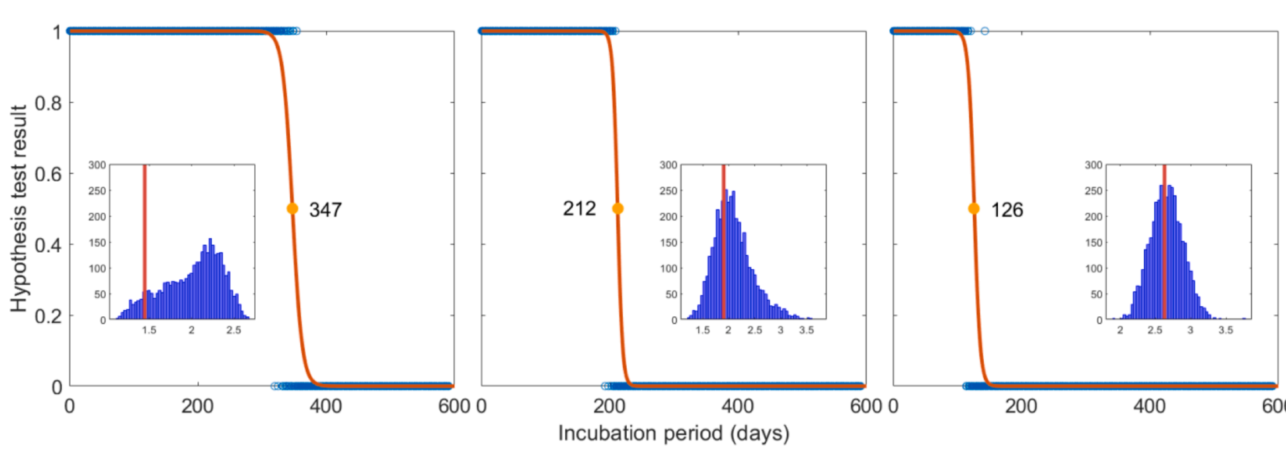

Fig. 4. T-test of difference between model predictions and synthetic data at day 600 when different lengths of incubation data were used under 15 °C (a), 25 °C (b), and 35 °C (c). H equals 1 when model predictions were significantly different from synthetic data at day 600, otherwise H equals 0. Logistic regression was performed to get optimal duration, where the second derivative of the fitted line equals 0 (yellow dot). The inset graphs illustrate the frequency distribution (x-axis) of model prediction (y-axis) at day 600 when 200 days of incubation data were used. The red line represents 'observation' at day 600.

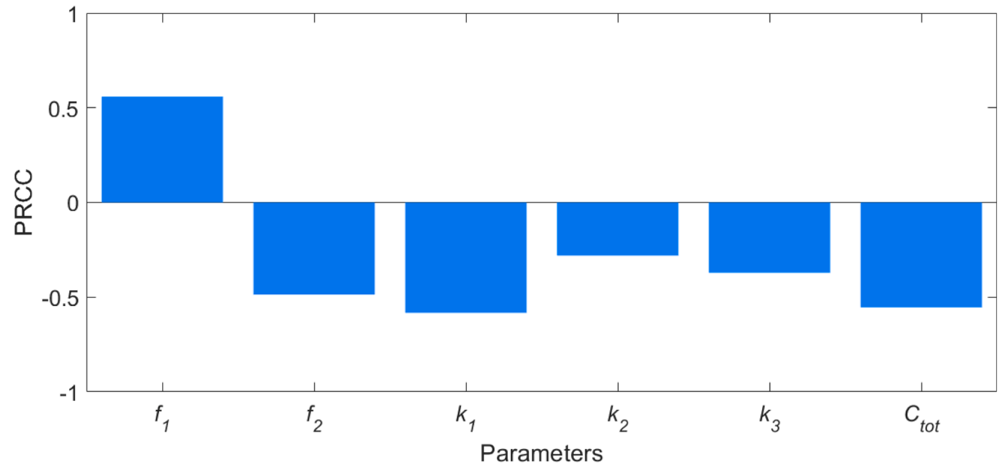

Fig. 5. Partial Rank Correlation Coefficient (PRCC) of optimal incubation period and parameters. Notations of the parameters are shown in Table 1.

turnover pool were incorrectly attributed to slower pools. As incubation experiments continue, the contribution of slow- and passive-turnover pools gradually increases (Fig. S4), and thus improves model predictability. Our sensitivity analysis further implied that a longer duration of incubation is needed for soils with a larger proportion of slow turnover pools (Fig. 5). Using the OPID approach during the experiment could reduce the uncertainty caused by short incubation duration.

The progressive data assimilation algorithm we developed could be used to forecast CO_2 emission from SOC decomposition for on-going incubation experiments. If forecasting of CO_2 emission becomes stabilized with adding incubation data, one would decide to stop their incubation experiment. Using synthetic data, our study eliminated experimental errors that would influence data assimilation and model projections. Data quality, frequency, and length of the observed data play a large role in estimating model parameters (Luo et al., 2009). In practice, experimental errors and data quality may result in higher RMSE, which implies longer incubation periods are needed than we expected. Further studies should be investigated to explore how data quality affects the optimal duration. However, we suggest using the average RMSE of the last 10 days to determine when it is appropriate to stop the incubation experiment. Take 35 °C as an example, after 126 days, the difference between the two days of RMSE was less than 0.05, which means the additional incubation data no longer contributed significantly to the decline of RMSE. Our algorithm could be integrated into the online interactive model-data fusion systems such as EcoPAD (Ecological Platform for Assimilation of Data) and PEcAN (The Predictive Ecosystem Analyzer). Models could be improved through updated data as well as guides the method of data observed (Huang et al., 2019). Experimenters could decide the length and frequency of data collection based on the model prediction when using those systems.

4.2. Factors influence optimal duration

While the accuracy of model projections increases with incubation period, their response patterns are different among different temperatures and exhibit a trade-off between initial model performance and the time towards accurate projection. That is, when the incubation period is relatively short, e.g., 60 days or shorter, the model performs better under lower temperatures than higher temperatures. In contrast, the relative performance switches with increasing incubation period. At the very beginning of an incubation experiment, data collected from CO_2 emissions were largely from the decomposition of the active fraction of soil carbon (Zou et al., 2005). At that time point, all three parameters would be overestimated and contribute to the overall overestimation of decomposition. The slow and passive pools are more sensitive to temperature than the active pool (Zhou et al., 2018). Therefore, under higher temperature, more CO_2 emission from slower pools would result in bias of parameter estimations. As the model can easily mistake CO_2 from slow pools for active pool, at the beginning of incubation experiment (Li et al., 2013). That is why we need to be more careful about experiment duration to determine whether we are getting enough information. As the experiment progresses, the decomposition of the slow and passive carbon pools begin to dominate. When feeding these data into a model, the model performance could increase dramatically. Under lower temperature, the slow and passive carbon pools still decompose slowly due to lower microbial activities. However, at higher temperatures, microorganisms are more active, and CO_2 emission data contains more mineralization information of the slow turnover carbon pools (Li et al., 2013; Wang et al., 2014). Therefore, the model performance under higher temperature increases faster than under lower temperature.

Our sensitivity analysis indicated that the optimal duration was influenced by soil properties that were related to SOC decomposition rates, fractions of different components, and the initial carbon content. The higher the mineralization rate was, the earlier the sufficient information of each pool was obtained, and the model could sooner achieve precise projections. Factors such as clay content, C:N ratio, and field water holding capacity (WHC), which affect decomposition rates and, therefore, the optimal duration of the experiment (Xu et al., 2016). The soil with high clay content may have more SOC been protected and recalcitrant to decomposition (Kölbl and Kögel-Knabner, 2010; Krull et al., 2001), which is reflected in the model parameters as decreased values of k_1 and k_2. The C:N ratio directly controls the nitrogen(N) availability for decomposers and WHC governs microbial decomposition and oxygen supply by influencing the soil water availability(Schjønning et al., 1999). Both of these factors may affect the decomposition rates, and influence optimal duration of the experiment indirectly. The proportion of SOC fractions will also influence optimal duration. If there is more active carbon in SOC (large f_1), the duration that the active pool acts as the major pool to release CO_2 is longer. Therefore, the model has difficulty in catching more information on the slow and passive pools from the short-term incubation data and needs more time to make precise predictions. It was a surprise that soil with higher carbon content could reach optimal duration earlier, despite that soil with a higher carbon content needs more time to decompose. Incubation of soils with higher carbon content will produce larger CO_2 emission, which may provide enough information for data assimilation and precise prediction. Overall, our results implied that any soil properties that result in less information on the slow and passive pools, or more information on the active pool, would lead to larger predicted deviations and would need a longer incubation period.

To consider differences between sampling frequency of synthetic and real data and to further test the contribution of sampling frequency to model parameters, we changed the daily synthetic data to four different sampling frequencies: every 3 days, weekly, bi-weekly, and monthly. We ran the OPID approach following the steps in the methods, then compared the parameters posterior distribution and the range of the estimated values (Fig. S6). We found that the uncertainties of parameters estimation from the incubation durations of 30, 100, 200, and 365 days changed slightly with sampling frequency. The reduced frequency increased parameter uncertainty, and this phenomenon was only obvious in the active pool with a 30-day incubation duration. However, the range of estimated values in k_2 and k_3 was not influenced by the sampling frequency. In addition, the peak of each distribution did not skew so that the sampling frequency did not influence the estimation of parameters value. The added test implied that the sampling should be highly frequent during the first 30 days of the incubation experiment to reduce the uncertainty of the active pool.

Uncertainty of model structure might influence the performance of our approach. There are a number of models for soil organic carbon decomposition, such as CENTURY model(Parton et al., 1987), RothC model(Coleman and Jenkinson, 1996), and DocMod model(Currie and Aber, 1997). In this study we used the classic three-pool model, in which different pools were separated according to their decomposition rate. Recent developments on SOC stabilization mechanisms explained that SOC with physical protection or with chemical recalcitrance was defined as slow pool, and that with mineral protection was defined as the passive pool (Chen et al., 2021). Our three-pool based model still persist for those SOC stabilization as long as three SOC pools can be defined. Microbial communities could regulate decomposition rate of SOC. There developed microbial-explicit models such as MEND model (Wang et al., 2015), MESDM model (Zhang et al., 2022), aim to capture decomposition patterns mediated primarily by saprophytic microorganisms such as microbial dormancy, microbial functional groups, priming effect. However, including nonlinear microbial process could result in oscillation of CO_2 release, which can not realistically represent soil carbon dynamics (Wang et al., 2016). In addition, microbial-explicit models have more parameters than first-order kinetic models, and therefore increase the parameter uncertainty. If future advances in experimental techniques that could monitor soil fraction data through incubation, other complex models could be tested.

5. Conclusion

In summary, the OPID approach developed in this paper utilized incubation data to effectively determine the optimal duration of an incubation experiment. Our approach can make predictions on SOC mineralization after the incubation begins, but a longer period was needed to constrain the parameters. Researchers can decide when to terminate the experiment according to the purpose of their research. In future studies, to efficiently design an experiment, a range of simple to complex soil C decomposition models could be tested with our progressive data assimilation approach.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

R script is uploaded

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.geoderma.2022.116225.

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