Thank you for your careful explanations and revisions, including fixing the errors that we didn’t see in the first place. In general I find the manuscript now ready for publication.

Thank you. We have made the suggested adjustments to the manuscript, as described below.

Thank you for taking the time for investigating the origin for the apparent misunderstandings. You are right the term you use to represent the $Z_p$ parameter as text was, and is still, confusing. Both ‘depth of production’ and ‘e-fold depth of production’ ($= \text{depth of production times } e^{??}$). It should rather be height at $1/e$ of total production, shouldn’t it?) are in my opinion still not exceptionally well suited. These terms imply other meanings than simply describing a parameter that scales a vertical distribution function (maybe you should call it scaling parameter $Z_p$?). Anyway, if there is no better solution, I suggest simply defining $Z_p$ as you did, explaining it once and then using the symbol all the way through.

As suggested, the symbol $Z_p$ has replaced the term “e-fold depth of production” in the majority of instances throughout the article. The term “e-folding depth of production” is still used in the definition of the $Z_p$ variable, as it appears to be the most commonly used term in related articles. A quick search on Google scholar returned 250+ articles using this term in soil studies, significantly more hits than other options such as “depth of production” (154) and “characteristic production depth” (10). As “e-folding depth of production” has been the dominant term used in other studies to describe the same concept that we’re describing, using it here would likely be beneficial to reader understanding.

Although a plausible claim, as you demonstrate with the references to previous work, it is still hypothetical that the chosen vertical distribution function is actually representing the CO2 production in a real world soil correctly. In a real soil the specific vertical distributions of SOM content in general and litter content specifically and of soil water contents, soil textures and not to forget roots may compromise the match with exponential shape and the model inversion will probably compensate for the inconsistencies between reality and the shape function by biased parameter values. I’m happy that you emphasised this reasoning in the discussion and in the conclusions.

Yes, the vertical distribution function of CO2 production would certainly be site
specific. Users of this inversion method would ideally have a measurement-based estimate of the vertical distribution at their particular site; otherwise additional errors may be incurred. Thank you for pointing out the need for clarification on this matter.

So my last wishes for changes are:

1. change ‘e-fold depth of production’ preferably as suggested above

   **Thank you. Fixed.**

2. To avoid misunderstandings: when speaking of parameters it is always a challenge to make clear whether one means the term (e.g. parameter Q10) or its value (i.e. the Q10 value). In your text you, e.g., write ‘different Q10s’ (e.g. track changes version line 180), or ‘to determine depth-specific Q10’ (line 410). To make clear that you mean the values and not the parameter per se, rather use Q10 values – i.e. specific Q10 values

   **Fixed, thank you for pointing out this possible source of confusion.**

3. 430 remove certainly

   **Thank you. Fixed.**

   **We hope that these minor changes have added to the overall cohesiveness of the text. Thank you for your time, comments and consideration.**
An inversion approach for determining distribution of production and temperature sensitivity of soil respiration

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Abstract. Physical soil properties create lags between temperature change and corresponding soil responses, which obscure true Q_{10} values and other biophysical parameters such as depth of production. This study examines an inversion approach for estimating Q_{10} and e-folding depth of CO_2 production (Z_p) using physically based soil models, constrained by observed high-frequency surface fluxes and/or concentrations. Our inversion strategy uses a 1-D multi-layered soil model that simulates realistic temperature and gas diffusion. We tested inversion scenarios on synthetic data using a range of constraining parameters, time averaging techniques, mechanisms to improve computational efficiency, and various methods of incorporating real data into the model. Overall, we have found that with carefully constrained data, inversion was possible. While inversions using exclusively surface flux measurements could succeed, constraining the inversion using multiple shallow subsurface CO_2 measurements proved to be most successful. Inversions constrained by these shallow measurements returned Q_{10} and Z_p values with average errors of 1.85% and 0.16% respectively. This work is a first step toward building a reliable framework for removing physical effects from high frequency soil CO_2 data. Ultimately, we hope that this process will lead to better estimates of biophysical soil parameters and their variability on short timescales.

1 Introduction

Soil respiration, which includes both root and microbial respiration, represents the largest outward flux of CO_2 from terrestrial ecosystems, with a magnitude far above that of anthropogenic emissions [Raich and Schlesinger, 1992]. Small changes in the soil CO_2 flux could therefore have a significant impact on the carbon balance and global atmospheric CO_2 concentrations. In predictions of atmospheric CO_2 over the 21st century, uncertainties surrounding the response of land flux to
Climate change are second only to uncertainties surrounding future anthropogenic emissions (Meir et al., 2006). In order to accurately predict future atmospheric CO\textsubscript{2} concentrations, it is crucial to gain a better understanding of how land systems will respond to changing temperature and moisture regimes.

Soil CO\textsubscript{2} production originates from plant root respiration and microbial decomposition of organic matter. The temperature sensitivity of soil respiration describes how the flux of CO\textsubscript{2} from soils will respond to a change in temperature. Normally soil microbial and plant root processes are treated together because they are not readily distinguished from one another. Temperature sensitivity is often quantified by a parameter Q\textsubscript{10}, which describes the factor increase in soil respiration with a temperature increase of 10\textdegree C. This Q\textsubscript{10} parameter is used in global climate models to quantify soil feedbacks to climate change. It has been found that Q\textsubscript{10} values are influenced by a range of environmental factors including soil temperature (Lloyd and Taylor, 1994; Luo et al., 2001), soil volumetric water content (Davidson et al., 1998; Reichstein et al., 2002) and soil organic matter content (Taylor et al., 1989; Wan and Luo, 2003). As these factors exhibit high spatial heterogeneity across ecosystems as well as within a given ecosystem, it has long been expected that Q\textsubscript{10} will also exhibit high spatial variability. Despite this, most existing models continue to use a globally constant Q\textsubscript{10} value. This may reduce or enhance predicted release of CO\textsubscript{2} from soils, leading to large over- or under-estimates of the contribution of soil respiration to terrestrial CO\textsubscript{2} flux in the face of climate change. There has been considerable debate over the usage and magnitude of Q\textsubscript{10} (Davidson et al., 2006; Mahecha et al., 2010), with different studies producing widely variant values. While most studies agree that CO\textsubscript{2} flux feedback will be positive, there is no consensus on how best to estimate the magnitude of Q\textsubscript{10}.

Historically, Q\textsubscript{10} values have been determined through regression analysis of soil temperature and CO\textsubscript{2} surface flux measurements. A known source of error in this approach originates in the physics of soil heat and gas transport, which might separate a change in surface soil temperature (normally a 5 cm or 10 cm temperature is used for deriving Q\textsubscript{10}) from the resultant change in CO\textsubscript{2} flux measured at the surface. The lags depend most heavily on soil heat transport (Phillips et al., 2011), because changes in surface temperature are shifted and dampened significantly as a function of depth, with each successive soil layer experiencing a reduced temperature change in amplitude. Gas diffusion also plays an important role, and even if soil microbes and roots produced CO\textsubscript{2} instantaneously upon receipt of thermal energy at the characteristic production depths, gases still take time to diffuse upward. Soil properties including heat and gas diffusion, and the e-folding depth of CO\textsubscript{2} production (Z\textsubscript{p}), all contribute to these lags (Fig. 1). Phillips et al. (2011) demonstrated that such lags can lead to severe misinterpretation of data when attempting to extract true Q\textsubscript{10} values through regression of surface flux and a temperature measurement at a single depth.

These thermal and gas diffusion processes, and the resulting lags, can be captured in a simple 1-D physical heat and gas transport soil model (Nickerson and Risk, 2009; Phillips et al., 2011).
Though not done to date for the soil respiration system, it is possible to use such a model in inverse fashion for estimating the value of parameters like $Q_{10}$ and $Z_p$ by looping the forward model iteratively through possible parameter combinations, with observed measurements as a constraint. Normally, an objective function is used for helping decide which parameter set best minimizes the difference between modelled and measured data. This method has been identified as a promising tool for determining unknown soil parameters (Zhou et al., 2009), with an increasing availability of high frequency data sets allowing for rigorous constraints on known model parameters.

This study seeks to develop a reliable inversion framework for determining the $Q_{10}$ and $Z_p$ of different sites given continuous soil measurements. It also seeks to provide guidance for researchers who would like to build field observational sites suited for inversion analysis. Working exclusively with synthetic soil data that mimics the form of collected field data and of which all parameters are known, we first undertake sensitivity tests to determine optimal sensor placing in the field, and decide whether soil CO$_2$ surface flux, and/or profile measurements, are more suited for anchoring inversion approaches with the necessary field data for parameter constraint. Using the best sensor combination, we are able to evaluate the accuracy of the inversion approach in returning the original $Q_{10}$, and $Z_p$, across many realistic soil type scenarios.

2 Methods

This study uses a one dimensional CO$_2$ and heat transport model described by Phillips et al. (2011), originally developed by Nickerson and Risk (2009). This model, with existing versions in Perl and R (R Core Team, 2015), was recoded in C to increase computational efficiency for the parameter solving routine.

2.1 Model description

This model (Fig. 2) simulates the movement and production of CO$_2$ through the soil profile and into the free atmosphere. The model consists of one atmospheric layer and a soil profile 1 m in length, divided into 100 layers of uniform thickness. Each layer can exchange CO$_2$ with its two nearest neighbouring layers using the 1-D discrete form of Fick’s first law:

$$F_{ij} = -D_{ij} \frac{\Delta C_{ij}}{\Delta z_{ij}}$$

where $D_{ij}$ is the effective diffusion coefficient between two soil layers, $\Delta C_{ij}$ is the CO$_2$ concentration difference ($\mu$mol m$^{-3}$) and $\Delta z_{ij}$ is the difference in depth (m) between the two layers.

For every modelled time step, each soil layer has a defined temperature, biological CO$_2$ production, CO$_2$ flux, thermal diffusivity and gas diffusivity. Temperature varies sinusoidally on daily and annual timescales. Changes in surface temperature are shifted and dampened through the soil profile
using:

\[ T[i] = T_{avg} + \Delta T_D e^{\frac{-z_i}{d_{Td}}} \sin \left( \omega_D t - \frac{-z_i}{d_{Td}} \right) + \Delta T_Y e^{\frac{-z_i}{d_{Ty}}} \sin \left( \omega_Y t - \frac{-z_i}{d_{Ty}} \right) \]  

(2)

\[ d_{Td} = \sqrt{\frac{2D_T[i]}{\omega_D}}, d_{Ty} = \sqrt{\frac{2D_T[i]}{\omega_Y}} \]  

(3)

which simulates the lags related to the rates of thermal diffusion. In this equation, \( T_{avg} \) is the average temperature in the air and soil profile for the duration of the simulation, \( \Delta T_D \) is the amplitude of the daily temperature fluctuation, \( \Delta T_Y \) is the amplitude of the yearly temperature fluctuation, \( \omega_D \) is the radial frequency for daily oscillations (\( \omega_D = \frac{2\pi}{86400} \) s), \( \omega_Y \) is the radial frequency for annual oscillations, \( z_i \) is the layer depth (m), and \( D_T \) is the thermal diffusivity of the soil (m\(^2\) s\(^{-1}\)).

Biological CO\(_2\) production in each layer is calculated using an exponentially decreasing function \(^{(Nickerson and Risk, 2009)}\):

\[ P[i] = \frac{\Gamma_0}{\sum_{i=1}^{N} e^{\frac{-z_i}{Z_p}}} Q_{10}^{T[i] - T_{avg}} e^{-\frac{z_i}{Z_p}} Q_{10}^{T[i] - T_{avg}} \]  

(4)

where \( \Gamma_0 \) is the total basal soil production (\( \mu \)mol m\(^{-3}\) s\(^{-1}\)), \( N \) is the number of soil layers, \( Q_{10} \) is the temperature sensitivity of soil respiration, \( z_i \) is the depth of the layer (m) and \( Z_p \) is the e-folding depth of CO\(_2\) production (m), defined as the depth below which the total fraction of CO\(_2\) production remaining is 1/e (also called the damping depth characteristic production depth in some studies), from which the production at any depth \( P(i) \) can be calculated based on equation 4.

Initially, the diffusivity of CO\(_2\) in the soil profile is calculated using the Millington Model \(^{(Millington, 1959)}\), an empirically derived approximation for calculating diffusivity in the field:

\[ D_c = \frac{\theta_w D_{fw} + \theta_g D_{fg}}{\theta_T^2} \]  

(5)

\( D_{fw} \) and \( D_{fg} \) are the diffusivity of CO\(_2\) in free water and free air (m\(^2\) s\(^{-1}\)), \( H \) is the dimensionless form of Henry’s solubility constant for CO\(_2\) in water, and \( \theta_w, \theta_g \) and \( \theta_T \) are the water filled, air filled and total soil porosities, respectively.

At each time step, the diffusivity of each soil layer is calculated using a temperature correction on this Millington diffusivity:

\[ D[i] = D_c \left( \frac{T[i]}{T_{avg}} \right)^{1.75} \]  

(6)

As previously mentioned, the flux from each layer is determined by Fick’s first law, written explicitly as:

\[ F[i] = D[i] \left( \frac{C[i] - C[i-1]}{dz} \right) dt \]  

(7)
where $C[i]$ is the CO$_2$ concentration of layer $i$ ($\mu$mol m$^{-3}$), $C[i-1]$ is the concentration of the layer above, and $dt$ is the time step (s).

Finally, at each time step CO$_2$ concentration in each layer $i$ is calculated using:

$$C[i] = \frac{C_{t-1} \theta_g dz - F[i] + F[i+1] + P[i]}{\theta_g dz}$$

(8)

where $C_{t-1}[i]$ is the layer concentration at the previous time step, $F[i]$ is the flux of CO$_2$ leaving layer $i$, $F[i+1]$ is the flux of CO$_2$ entering the layer from the layer below, $P[i]$ is the CO$_2$ production within layer $i$.

### 2.2 Model execution and validation

Before beginning the simulation, the system is initialized using input parameters seen in Table 1. Atmospheric CO$_2$ concentration remains constant for the duration of the simulation; it is assumed that any flux from the soil will quickly dissipate into the atmosphere. Flux from the bottom soil boundary is set to zero, as production at this depth is negligible according to the exponentially decreasing production function. These system parameters were changed depending on the soil type being simulated.

After initialization, the system undergoes spin-up, during which layer temperatures are held constant at their initial values, and the model is run until the CO$_2$ concentration in each layer is constant. The duration of the spin up period is dependent on soil diffusivity (and therefore $\theta_w$), and is determined by plotting concentration vs time through the soil profile. This period ranges from 5 to 23 model days within the range of $\theta_w$ (0.1 to 0.25). The CO$_2$ concentration in each layer after spin up is the initial layer concentration at the beginning of the actual simulation.

For each modelled time step ($dt=1.0$ s), temperature, CO$_2$ diffusivity, CO$_2$ production and CO$_2$ flux are calculated in each soil layer. Every soil layer is then revisited, and the new CO$_2$ layer concentrations are calculated. The progress of the simulation is monitored by outputting the CO$_2$ concentration and temperature of specified layers.

### 2.2.1 Validation

To ensure the model was performing correctly, steady state concentrations through depth (following spin-up) were compared to the steady state solution proposed by [Cerling (1984)](https://doi.org/10.1007/BF00361653). Daily and yearly temperature fluctuations were removed from the model, and the model was run until CO$_2$ concentrations in each layer were constant. Deviations of modelled from analytic concentrations were found to be far less than 1%.
2.3 Incorporating constraining data

In this study, we incorporated external data in the same way we would with field studies. We started with real measurements of temperature through depth, and soil volumetric water content, from a local field site. One of the largest challenges in preparing data for inversion is to accurately model soil temperature through depth and time, as temperature is the known determinant of soil lags (Phillips et al. 2011). For each set of temperature measurements through depth, a linear regression (in R) was performed, resulting in a 5th order polynomial for temperature through depth every 1800 s. A linear interpolation through time was performed to obtain temperature values in each layer for every modelled time step. The resultant temperature values replaced our originally sinusoidally varying temperature function in the model. The value of thermal diffusivity was therefore implicitly built into these measurements and is no longer required as a direct model input.

These physical variables were used in a forward instance of the soil model to create CO$_2$ surface flux and CO$_2$ concentration timeseries. Datasets were created using many $e$-folding depths of production $Z_p$ and $Q_{10}$ values of interest, so that we had many idealized datasets on hand in which concentration, fluxes, and associated temperatures, $e$-folding depths of production, $Z_p$ and $Q_{10}$ values, were known. Soil volumetric water content was not formally incorporated as a driver of respiration in these synthetic datasets, so all simulations were performed over periods of constant soil volumetric water content. During inversion we pretended not to know $e$-folding depths of production $Z_p$ and $Q_{10}$ values of these synthetic datasets, and hoped the inversion process would return the known values. Since the same forward soil model that generated the synthetic datasets was also embedded within the inversion scheme, errors in $e$-folding depth of production $Z_p$, or $Q_{10}$, would be due entirely to the inversion process itself.

2.4 Inversion process

The soil profile CO$_2$ concentrations and soil CO$_2$ surface flux are outputs of the simulation. Their values are dependent on all of the system input parameters. A method called inverse parameter estimation is employed to determine the values of $Q_{10}$ and $e$-fold depth of production $Z_p$ that would have given rise to the observed concentrations and fluxes. Through this process, model outputs are compared to measured field data or synthetic data over a range of model input parameters. The field measurements used in this process will be referred to as the model constraints; these constraints consist of CO$_2$ concentration measurements at various depths in the soil profile, as well as CO$_2$ surface flux measurements.

2.4.1 Inversion steps

The model is run for two unknowns, including $Q_{10}$ values ranging from 1 to 5.5 in steps of 0.1, and $Z_p$ from 0.02 m to 0.3 m in steps of 0.01 m. This results in a total of 1260 parameter combinations.
Inversion seeks to identify the parameter set that minimizes the objective function

\[
\sqrt{(S_1 - M_1)^2 + (S_2 - M_2)^2 + (S_3 - M_3)^2 + \ldots} \quad (9)
\]

where \(S_i\) and \(M_i\) correspond to modelled and measured CO\(_2\) concentrations at various profile depths. For each parameter set, this objective function is calculated every 1800 timesteps and averaged at the end of the simulation. The pair that minimizes Eq. (9) is output as the inversion result.

### 2.5 Validation of the inverse method

Before applying the inversion method to real field data, tests must be done to ensure method accuracy, and this manuscript focuses on such tests. We created synthetic timeseries using the original soil model, that mimic the form of real data sets. The values of \(Q_{10}\) and \(Z_p\) were known for each synthetic timeseries, as these parameters are required to run the model. This synthetic data included temperature measurements at six depths in the profile, volumetric water content, CO\(_2\) surface flux and CO\(_2\) concentration measurements at various depths in the soil profile.

The inverse method was applied to these synthetic data sets, and the output value of \(Q_{10}\) and \(Z_p\) could then be compared to the actual values of these parameters used to create the timeseries.

#### 2.5.1 Constraint, sensitivity, and random error testing

To determine which model constraints resulted in the highest accuracy of the inversion method, the error (Eq. (9)) was calculated using a large range of constraining parameters and combinations thereof. A total of 35 different constraint combinations were tested, representing various combinations of surface CO\(_2\) flux, and subsurface CO\(_2\) concentration measurements up to 0.6 m depth. These combinations are illustrated in Table 2. Testing which constraints consistently returned the most accurate values of \(Q_{10}\) and \(Z_p\) aids in determining optimal sensor placing the field.

To ensure model validity across all possible parameter values that may be encountered in the field, extensive sensitivity testing was done using these synthetic timeseries. These timeseries were created across a range of combinations of \(Q_{10}\), \(Z_p\), volumetric water content (diffusivity) and total soil production. Table 3 illustrates the ranges tested for each parameter.

Field-deployable CO\(_2\) sensors typically have 1-5 % error. To see how the model and inversion would perform under these conditions, errors of 1, 5 and 10 % were added into all components of the synthetic data. The effect of these errors on the inverse method were observed.

### 3 Results and discussion

Inversions on synthetic timeseries were successful across all tested soil parameters, though some CO\(_2\) concentration measurement depth combinations (surface flux, single or multiple profile measurements) helped to minimize the overall error, as well as the error in \(Q_{10}\) and \(Z_p\) individually.
Errors discussed in this section represent an average from 64 inversions across values of $Q_{10}$, e-fold depth of production $Z_p$, and soil diffusivity as presented in Table 3. In this section, we use either fractional error ($\frac{|\text{actual} - \text{result}|}{\text{actual}}$), or absolute deviation from the actual value ($|\text{actual} - \text{result}|$).

3.1 Best measurement configurations to obtain $Q_{10}$ and $Z_p$ via inversion

In Fig. 3 we show the average fractional error in the returned $Q_{10}$ value for every combination of subsurface CO$_2$ sensor measurements. Observations of CO$_2$ concentration shallow in the soil were found to be necessary for highly accurate $Q_{10}$ estimates. The lowest inversion error for $Q_{10}$ was 1.85%, in a scenario where subsurface measurements were made at 5, 10 and 15 cm. Single concentration measurements at or above 10 cm also proved successful, with errors < 2.3 %. The least accurate inversions for $Q_{10}$ occurred when the constraint consisted of (single or multiple) CO$_2$ concentration measurements deep in the soil profile. We propose that the poor performance of inversion when using deep profile constraints could be related to the low magnitude of thermal and concentration variability at these depths. Deep soil layers are subject to much smaller thermal fluctuations than layers close to the surface. In this less variable environment, CO$_2$ concentrations are less variable and provide less of a signal upon which to anchor inversion. In contrast, CO$_2$ concentrations shallow in the soil exhibited larger variations in temperature and concentration, which presumably allowed $Q_{10}$ to be extracted more easily. If the primary interest is to obtain $Q_{10}$ from inversion, multiple CO$_2$ concentration measurements in the soil were found to be important. It should be noted that, while differences in error rate were noted, errors for all scenarios could be considered tolerably low relative to the normal variance expected from regression-based $Q_{10}$, considering the gas transport lags inherent in those data (Phillips et al. [2011]).

The average fractional error in $Z_p$ for different model sensor combination constraints is also shown in Fig. 3. Out of the 35 combinations tested, only 5 resulted in an average $Z_p$ error greater than 2%. Single concentration measurements shallow or deep in the soil profile caused this larger error, but on average, single concentration measurements at any depth in the soil were less accurate. Inversions constrained by at least one measurement shallow (< 15 cm) and one deep (≥ 30 cm) in the profile returned $Z_p$ with 100% accuracy across all sensitivity tests. We did expect that single measurements deep in the profile would perform poorly relative to others, because with the exponentially decreasing production defined in the model, CO$_2$ production approaches zero at significant depths regardless of the value of $Z_p$ and thus cannot perform well as an inversion anchor. The large $Z_p$ error of almost 25% associated with soil surface CO$_2$ flux measurements, was also not surprising. In this situation the inversion scheme must reconstruct $Z_p$ mainly via the temporal delay, and damping, between sinusoids of temperature through depth, and soil surface CO$_2$ flux. Without a concentration measurement in the soil, the gas transport regime is black boxed from the perspective of the inversion scheme, resulting in the large error. Overall, surface CO$_2$ flux measurements alone are less suited
for elucidating information on e-folding depth of production, whereas a combination of shallow and deep measurements is best for reconstructing the distribution of CO$_2$ production in the soil profile.

In examining inversion accuracy for both parameters $Q_{10}$ and $Z_p$ simultaneously (Fig. 3), we found that multiple concentration measurements shallow in the soil ($\leq 15$ cm), or combinations shallow in the soil with one deep concentration measurement ($\geq 30$ cm) were the best constraints. Deep soil measurements and surface flux constraints should therefore be avoided if the aim is the minimize overall error. This overall result is a combination of what was found for $Q_{10}$ and $Z_p$ individually, where shallow measurements were best for $Q_{10}$ and a combination of shallow and deep measurements resulted in most accurate $Z_p$.

Depending on error tolerance for the final parameter estimates, it is conceivable that the accuracy of all inversions performed here might be sufficient for the community of soil scientists. Out of the 35 combinations tested, 19 resulted in an overall average error less than 5%. The top constraint (measurements at 5, 10 and 15 cm) had an average error of 2.01%, and the top 6 combinations all had error less than 3%. These errors are small compared to the degree of random error in CO$_2$ flux studies (Lavoie et al., 2015). These results are summarized in Table 4, where the top and bottom 5 combinations are listed individually and overall.

This assessment was performed using synthetic data, and even the most ideal field settings will depart from these modelled profiles. For example, we represented CO$_2$ production through depth using an exponential production function, but a field site may show a linear decrease in production at increasing depths. Clearly users of the inversion process will want to characterize as many site-specific parameters as possible so as to provide proper guideposts and constraints for the inversion, otherwise additional error will be introduced. The sensitivity of the inversion to error is an important question, and will be addressed in a later section.

### 3.2 Effect of soil-specific parameters on inversion success

Having determined the best CO$_2$ sensor concentration measurement depth to constrain inversions, we can examine how site-specific parameters such as soil diffusivity, depth of CO$_2$ production $Z_p$ and $Q_{10}$ affect inversion results. For this assessment, we will use the best performing measurement configurations established. Even when not a top choice, we will always include CO$_2$ surface flux measurements in this section, because of the likelihood that scientists will want to use inversion to analyze these data which are increasing in number rapidly.

Figure 4 a) and b) illustrate how deviation in $Q_{10}$ and $Z_p$ were affected by the diffusivity of soils. When subsurface sensor combinations were used as a constraint, there was an overall downward trend in $Q_{10}$ and $Z_p$ error with increasing diffusivity. As diffusivity increases (drier soils), CO$_2$ travels through the soil layers to the surface more quickly which results in decreased lag times, more rapid concentration changes, and more distinct soil responses. Under these conditions of rapid diffusion, inversions were most successful. Sites that are frequently waterlogged with limited air
filled pore space tended to be less ideal for inversion, but the optimal instrument configuration still helps ensure reasonably small error throughout the entire range of diffusivities, so there is no strict limitation on the use of the inversion approach in low diffusivity soils.

Figure 4 c) and d) demonstrate the impact of the Zp parameter value on inversion success in terms of deviation in returned Q_{10} and Zp values. For small Zp values, shallow CO₂ concentration measurements (≤ 15 cm) were the best constraints, presumably because the soil is most active in these top layers. As e-fold depth of production Zp increases, the production of CO₂ is no longer limited to the shallow soil, the exponential production function decreases more slowly. With increasing Zp, CO₂ production in deeper soil layers is higher, and more useful as an inversion constraint. Some matching of deployment depth was also found, where for example shallow concentration measurements were more accurate for returning the correct value of shallow CO₂ production.

Sensitivity tests indicate that increasing the temperature sensitivity of respiration had opposite effects on Q_{10} and Zp error. Deviation in returned Q_{10} values increased rather uniformly across the best subsurface measurements, while for most subsurface combinations the Zp error decreased. With increasing Q_{10}, respiration becomes more sensitive to temperature changes, leading to larger variations in production in the event of a temperature fluctuation. Figure 4 e) and f) illustrate the impact of this parameter on Q_{10} and Zp error.

With large amounts of existing surface flux data, it is also worth examining the effectiveness of the soil CO₂ surface flux as a constraint, even when it is not the preferred constraint. It is immediately evident from Fig. 4 that inversions constrained by the surface flux resulted in Q_{10} and Zp deviations that responded much differently to changes in soil diffusivity, e-fold depth of production Zp and Q_{10}. These deviations were often significantly larger than when subsurface constraints were used. Deviations in Q_{10} and Zp generally increased as all three parameters increased. This suggests that for low diffusivity, e-fold depth of production Zp and Q_{10}, surface flux was a reasonable model constraint, producing errors comparable to the subsurface measurements. This constraint was much less effective for determining depth of CO₂ production. However, Zp was always returned within at least 3.5 cm of its actual value, which for some uses may be an acceptable level of uncertainty. Inversions constrained by surface flux were quite effective in returning Q_{10}. Returning to Fig. 3, the overall average Q_{10} error associated with surface flux was less than 5%, which is significantly better than results using deep subsurface measurements. Figure 4 e) suggests that inversions using large Q_{10} values were responsible for the majority of this error. For Q_{10} of 1.5, these inversions returned Q_{10} with 100% accuracy. For the largest Q_{10}, deviation from the true value climbed as high as 0.6-0.7, which is non-negligible. A shorter model time step could potentially reduce this error, as it may be able to better capture the larger and faster responses associated with high Q_{10} and diffusivity. As we cannot estimate the Q_{10} of a site prior to inversion, however, this insight may not be overly useful in site selection. Overall, inversions constrained by the CO₂ surface flux are possible but should be performed with caution, and with reasonable expectations as to the resultant error level.
It is also of interest to examine how the amount of CO$_2$ production in the soil profile affects inversion. The bulk of our sensitivity tests were performed using a basal CO$_2$ production of 10 $\mu$mol m$^{-3}$ s$^{-1}$, which is a fairly high. In order to test the other extreme, several inversions were performed using a production level of 1 $\mu$mol m$^{-3}$ s$^{-1}$. These inversions performed with exactly the same accuracy as those with a production level of 10. From this, we can conclude that the magnitude of production has no effect on inversion success.

3.2.1 Random error and inversion

The measurements performed by sensors in the field will always be uncertain to some degree. It is therefore important to examine how these uncertainties in recorded temperature, CO$_2$ and soil volumetric water content measurements will impact the accuracy of the inversion method. Inversions performed on synthetic data to which random errors of 1, 5 and 10% had been added were indeed less accurate than those performed on idealized data. However the resulting errors in returned $Q_{10}$ and $Z_p$ were not proportional to the amount of error added to the input data, but actually much lower. That is, errors of 5% in the input data did not result in an additional 5% error in output values. An example of this is illustrated in Fig. 5. This plot demonstrates that with random measurement errors in the ranges of 1-5%, $Q_{10}$ values were still determined with reasonable accuracy. Prior to error addition, deviation in $Q_{10}$ was around 0.12. This deviation increased to 0.14 for 1% error and 0.17 for 5% error. As sensors in the field are typically uncertain by 1 to 5% , the inversion method remains feasible. We can thus conclude that the inversion process is rather tolerant of error in measurement.

3.3 Multi-parameter error landscape

It is worth investigating in detail the error landscape of the inversion process using a multi-parameter sensitivity tests. For this test, we chose the combination of measurements at 5, 10 and 15 cm which had resulted in the most accurate inversions on average.

The results from the sensitivity tests are shown in Fig. 6, panels a) to f). In all combinations, the error in $Z_p$ was very small, with the maximum error for any single inversion being just over 2%. Despite this small error, it remains evident which soil conditions should be avoided for most accuracy. Sites with low diffusivity, production deep in the soil and low $Q_{10}$ are the most problematic. This is consistent with the results from Fig. 4 a), c) and e). Trends were not as evident for error in $Q_{10}$. In panels a), e) and c) the most notable error was found in panel a) for high e-fold depth of production $Z_p$, low $Q_{10}$. There is an error in $Q_{10}$ here of almost 15%, which equates to a deviation in $Q_{10}$ of about 0.225 from its actual value. This result is not unreasonable, but it is significantly higher than results from the other inversions. Plot e) demonstrates an interesting result, where there seems to be a valley in the $Q_{10}$ error, illustrating a tradeoff between e-fold depth of production $Z_p$ and diffusivity. This is not evident in the other plots, and does not have an intuitive physical explanation. The effect of $Q_{10}$ on inversion varies, but success hinges quite clearly on soil diffusivity and depth.
of CO₂ production. Choosing a site in the appropriate ranges of these two parameters will maximize chances of success.

### 3.4 Limitations and opportunities

There are both limitations and future opportunities for the inversion approach. In general, the better an inversion is constrained with data, the better it will do in returning the true value for parameters of interest. Some of the soil parameters are distributed in ways that must be assumed. For example, the distribution of CO₂ production may be unknown. While most studies in the history of soil modelling have assumed an exponential distribution (and it has been seen in many studies using the gradient technique), some other considerations might help determine whether additional parameterization measurements are needed. For example, knowledge of rooting depth could be one aid. On average, root respiration accounts for 50% of soil respiration (Hanson et al., 2000 and Jackson et al., 1996) provide root distributions for different terrestrial biomes. Jackson et al. (1996) found that tundra, boreal forest and temperate grasslands had upwards of 80-90% of roots within the top 30 cm of soil whereas deserts and temperate coniferous forests had much deeper rooting profiles, with only 50% of roots within the top 30 cm. These and other methods may be helpful in providing constraint data when running inversions on real timeseries.

A future opportunity for inversion studies is to determine depth-specific Q₁₀ values, which would be of interest to many researchers. Currently there are few field examples where researchers have determined in-situ Q₁₀ as a function of depth, but two examples of such data using include gradient studies include Risk et al. (2008); Tang et al. (2003). Incubations might seem useful in this regard, but are disputed as a representation of in-situ conditions, especially at depth Risk et al. (2008).

Ideally, an inversion approach could determine depth-specific Q₁₀, but the reality is challenging. If an additional 100 Q₁₀ values were included as unknowns (one for each layer), it would increase computational demand by 100 times. The inversion results would also be confusing, and extreme values at one depth could potentially cause a spurious match to the measured data. The number of non-unique and implausible solutions would rise significantly as a result. A more reasonable approach might be to define Q₁₀ as we do e-fold Zₚ, which is as a function of soil depth. This would be computationally compact but whether a function would be realistic is not well known because there are so few examples of Q₁₀-depth profiles against which we could evaluate this approach. The best approach would be to use many profile concentration sensors for constraining data, so that the e-folding depth of production could be known, and the inversion could focus instead solely on determining layer-specific Q₁₀ values.

Despite the relatively nascent stage of our soil CO₂ inversion approach, indications are that it has better theoretical validity than traditional regression approaches, which do not take thermal- and gas-transport lags into account. Our error results here compare very favourably against error
analyses generated from detailed examination of regression approaches across thermal- and gas-
transport parameter space (Zhang et al., 2015; Phillips et al., 2011; Graf et al., 2008).

4 Conclusion

Overall, this inversion method proved successful in testing on synthetic data. Depending on the
tolerable level of error for a given application, almost every tested combination resulted in reasonably
accurate returned $Q_{10}$ and $Z_p$ values. The subsurface concentration measurements that yielded the
highest error were typically those that would be of least convenience to install and maintain deep
in the soil profile. The other constraint associated with high overall error was CO$_2$ surface flux,
which would likely be the data with highest availability. Most of the error from this constraint arises
in estimating the $Z_p$ parameter. The CO$_2$ surface flux is still a reasonable means of estimating $Q_{10}$
values via inversion. While in most cases the error was lower for high diffusivity, shallow production
soils, the application of this method is certainly not limited to such regions.

This method is computationally intensive as it performs a sweep through all possible combinations
in parameter space. This study used roughly 2.5 core-years of time despite the fact that synthetic
timeseries were short. This full sweep ensures that the global minimum in the objective function is
located every time, and when solving inversely for two unknown parameters (as we are), this is not
an unreasonable approach. However, if it was of interest in the future to examine longer timeseries,
or additional parameters such as the depth dependence of $Q_{10}$, resulting in additional unknown
parameters, it may be beneficial to explore other search algorithms to increase efficiency, such as
Simulated Annealing.

The next step for this work would be to perform inversions on real timeseries with appropriate
measurement constraints, to obtain temperature sensitivity and CO$_2$ production depth distribution
estimates for various sites. With the increasing availability of high frequency soil data, there would be
no shortage in data to analyze. Applying this method for periods of varying constant moisture levels
could also help build an understanding of moisture effects on temperature sensitivity of respiration.

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Nick Nickerson and Chance Creelman for valuable comments early on in this research.
References


Millington, R.J.: Gas diffusion in porous media, Science 130, 100-102, 1959.


Figure 1. Thermal and gas diffusion lags through a soil profile.
Figure 2. Conceptual representation of the 1-D layered soil model. Overall profile length is denoted with $L$, and $N$ represents the number of individual layers in the model soil profile.
Figure 3. Fractional Error in $Q_{10}$ and $Zp$ individually for different sensor combination scenarios, plus cumulative fractional error in $Q_{10}$ and $Zp$ for the same scenarios.
Figure 4. Error in $Q_{10}$ and $Z_p$ as a function of $Q_{10}$ (Panels C,F), $Z_p$ (Panels B,E) and D (Panels A,D), for a grouping of the best sensor measurement depth combinations. Individual 5 cm and 10 cm observational scenarios are shown in light blue and dark blue, respectively. The 5+15 cm measurement scenario is shown in green. Orange and red illustrate sensitivity of the 5+10+15 cm and 5+10+30 cm scenarios, respectively. Finally, the 4-point 5+15+30+60 cm measurement sensitivity is represented in grey while the surface flux scenario is shown in black. For these sensitivity tests, the known $Q_{10}$ was 2.0, and a $Z_p$ of 0.2 m was used.
**Figure 5.** Sample of random error effects on inversion, constrained by one concentration measurement at 5 cm. For this sensitivity test, the known $Q_{10}$ was 2.0.
Figure 6. Error in $Q_{10}$ and $Z_p$ as a function of $Q_{10}$, $Z_p$ and Diffusivity for the constraint 5+10+15 cm. For these sensitivity tests, the known $Q_{10}$ was 2.0, and a $Z_p$ of 0.2 m was used.
Table 1. Default parameter values for simulations

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<th>Parameter</th>
<th>Value/Range</th>
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<td>Soil porosity ($\theta_T$)</td>
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<td>Thermal diffusivity ($D_T$)</td>
<td>$5 \times 10^{-7}$ (m$^2$ s$^{-1}$)</td>
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<td>Average air and soil temperature ($T_{avg}$)</td>
<td>15°C</td>
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<td>Daily air temperature amplitude ($\Delta T_D$)</td>
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<tr>
<td>Yearly air temperature amplitude ($\Delta T_Y$)</td>
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<td>Atmospheric CO$_2$</td>
<td>380 ppm</td>
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<td>Total basal CO$_2$ production ($\Gamma_0$)</td>
<td>1-10 ( \mu \text{mol m}^{-2} \text{ s}^{-1} )</td>
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<td>Production exponential folding depth ($Z_p$)</td>
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<td>$Q_{10}$</td>
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<tr>
<td>Volumetric water content ($\theta_w$)</td>
<td>0.10-0.25 (v/v)</td>
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Table 2. Measurement combinations used for the simulations. The combination number is listed at the begin-
ning of each row. The columns represent the type of measurement (e.g. CO₂ surface flux), or the depth of
centimetre measurement in centimetres. The "X" values denote whether the type or depth of measurement
was included in the combination.

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Table 3. Default parameter values for sensitivity testing.

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<th>Abbr.</th>
<th>Minimum</th>
<th>Maximum</th>
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<td>Total basal CO₂ production (µmol m⁻² s⁻¹)</td>
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<td>Production exponential folding depth (m)</td>
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Table 4. Best and worst sensor combinations for determining Q₁₀, Zp and overall through inversion.

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