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Estimation of carbon transfer coefficients using Duke Forest free-air CO_2 enrichment data

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Abstract

A compartmental carbon model is presented in which there are parameters quantifying the transfer between various carbon pools. These parameters are estimated using two CO_2 data sets (elevated and ambient) from the Duke Forest FACE data set. A quadratic objective criterion is used to compare closeness of fit of system output CO_2 flux to the observed CO_2 flux data. Adjoint equations are developed based on the system of difference equations approximating the solution of the model equations, the data, and the criterion. Parameter estimation algorithms are developed using minimization techniques. It is found that the estimated parameters obtained using the two different data sets agree closely. © 2002 Elsevier Science Inc. All rights reserved.

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1. Introduction

The signing of the Kyoto Protocol requires the quantification of terrestrial carbon (C) sinks in various biomes [3]. The quantification has been done with both modeling and experimental approaches. Experimental studies have been conducted using open-top chambers and Free-Air CO_2 Enrichment (FACE)

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techniques to quantify the responses of terrestrial C sinks to elevated CO_2 [9]. Since forests are widely considered to have the largest potential among all the terrestrial biomes to act as sinks for atmospheric CO_2 [5], much effort is currently being directed towards studies of forest C uptake, storage, and release. At the Duke Forest in North Carolina, USA, a FACE facility has been installed since August 1996 to expose the mature forest canopy to an elevated level of atmospheric carbon dioxide [2]. Extensive measurements at the Duke Forest FACE site have provided many data sets for quantifying forest C fluxes. In order to predict the future rate of forests C sequestration, the data gained from the experiment need be used to quantify two keys parameters: gross primary productivity and residence time of C in the ecosystem [8]. The former is the amount of C that flows into the forest ecosystem via canopy photosynthesis and has been quantified with a canopy model [7]. The residence time of C in an ecosystem is determined by C transfer coefficients between pools [4].

This paper is to estimate C transfer coefficients at the Duke Forest using experimental data from the FACE experiment. Our mathematic analysis is based on the property of terrestrial C processes that transfers of the photosynthetically fixed C between pools usually follow a first-order linear function [6]. In Section 2 we describe pertinent features of the mathematical model and its approximation. The mapping that takes the solution vector of carbon pool sizes to the observed flux measurements is discussed in Section 3. Defining the estimation problem as a minimization problem of an object function that compares system outputs to the Duke Forest FACE data, in Section 4 the adjoint is introduced in order to calculate the derivative of the objective functional. Finally, in Section we report the estimated transfer coefficients for the ambient and elevated data sets to obtained close agreement in the estimated coefficients based on the two data sets.

2. The model equation and its approximation

We consider the nonautonomous linear system of $m = 12$ equations given by

$$x'(t) = A(t)x(t) + bu(t), \tag{1}$$

$$x(0) = x_0, \tag{2}$$

where the $m \times m$ matrix $A(t)$ is expressed by

$$A(t) = \tau(t)A_0C \tag{3}$$

for

$$A_0 = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.2877 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.7123 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.6664 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.3334 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.275 & 0.45 & 0.275 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.45 & 0.225 & 0 & -1 & 0.42 & 0.45 \\ 0 & 0 & 0 & 0.275 & 0 & 0.275 & 0 & 0.22 & 0.296 & 0.296 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.004 & 0.004 & 0.03 & -1 \end{bmatrix} \tag{4}$$

and

$$C = \mathrm{diag}(c), \tag{5}$$

where c is a column m-vector of weights that describe the exchange rates between various carbon pools. The solution vector $x(t)$ represents the vector of carbon pool sizes at time t. We use $\mathrm{diag}(c)$ to designate the diagonal $m \times m$ matrix whose entries along the diagonal correspond to the m-vector c. The functions $u(t)$ and $\tau(t)$ designate real numbers for each $t \in (0, T)$, the m-vector b is given by

$$b = \begin{bmatrix} 0.19 \\ 0.19 \\ 0.19 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}$$

and the initial value of pool sizes x_0 is given by

$$x_0 = [350\ 5000\ 220\ 230\ 70\ 500\ 70\ 230\ 160\ 135\ 3800\ 2500]'.$$

The function $u(t)$ gives carbon influx measurements of carbon entering the system. The function $\tau(t)$ is a product of two functions that give moisture and temperature measurements as functions of time. Under the assumption that u and τ are continuous functions t, it follows that there exists a unique solution, $x = x(c)$, of the initial value problem (1) and (2) for each m-vector c. Moreover, as a function of the parameter vector c, the mapping $c \mapsto x(c)$ is continuously differentiable [1].

Our purpose in this paper is to estimate the transfer vector c from the given data consisting of CO_2 flux from the Duke Forest FACE experiment. The data is in the form of a time series that we designate by $\{q_i^0\}_{i=1}^{N_0}$. To carry out this program requires several steps:

(i) For a given transfer vector c solve system (1) and (2) numerically to obtain an approximation of the pool size vector $x(c)$ associated with that transfer vector c.
(ii) Calculate the CO_2 flux as a system output $q(c)(t)$ associated with the transfer vector c. This is to be compared with observed measurement through a fit-to-data function. We express $q(c)(t)$ as a vector product of the pool size vector $x(c)$ with a convolution vector, $\phi(c)(t)$.
(iii) Define a fit-to-data functional $J(c)$ measuring the fit between the output $q(c)(t)$ and the observations $\{q_i^0\}_{i=1}^{N_0}$. This is a criterion by which we may judge the closeness of the system output and the data.
(iv) The transfer vector c we seek is a minimizer of the fit-to-data functional $J(c)$. To conduct the minimization, we use an iterative algorithm to adjust systematically the transfer coefficients in order to reduce progressively the value of the fit-to-data functional. The adjoint method is introduced to facilitate the calculation of the derivatives of $J(c)$ necessary to carryout this program.

In the remainder of this section, we develop a finite difference solution to the initial value problem (1) and (2). We also present the resulting set of difference equations in a form that is convenient for application later in developing adjoint equations for the minimization scheme. In Section 2 we give formulations of the observation in terms of a vector product and the estimation problem that lend themselves to mathematical treatment. The gradient of the fit-to-data functional in calculated in Section 3 by introducing the adjoint equations. This is done in order to update estimates of the transfer coefficients to reduce the value of the fit-to-data functional. Finally, in Section 4 the minimization algorithm is indicated and is tested using the Duke Forest FACE data with two sets of data. We find that the estimated transfer coefficients are essentially the same in both cases.

To solve numerically the above initial value problem, we introduce the uniform difference $\mathrm{d}t$ and let $t_j = j\mathrm{d}t$ for $j = 0, \ldots, N_T$ and set $x_j = x(t_j), A_j = A(t_j)$, and $u_j = u(t_j)$. Letting $\theta \in [0, 1]$, we introduce the difference equation

$$\frac{x_{j+1} - x_j}{\mathrm{d}t} = [\theta A_{j+1}x_{j+1} + (1-\theta)A_jx_j] + b[\theta u_{j+1} + (1-\theta)u_j]. \tag{6}$$

From Eq. (6) we obtain the recurrence equation

$$[I - \theta\mathrm{d}tA_{j+1}]x_{j+1} = [I + (1-\theta)\mathrm{d}tA_j]x_j + \mathrm{d}t[\theta u_{j+1} + (1-\theta)u_j]b. \tag{7}$$

For ease we define the matrices

$$B_j = I - \theta\mathrm{d}tA_j \tag{8}$$

for $j = 1, 2, \ldots, N_T$ and

$$\widehat{B}_j = I + (1-\theta)\mathrm{d}tA_j \tag{9}$$

for $j = 0, 1, \dots, N_T - 1$ and the column m vectors

$$f_i = \mathrm{d}t[\theta u_{j+1} + (1-\theta)u_j]b \tag{10}$$

for $j = 1, 2, \dots, N_T$. It is convenient to write the iterative system as collection of N_T equations

$$\begin{aligned}
&B_1 x_1 = f_1 + \widehat{B}_0 x_0 \\
&-\widehat{B}_1 x_1 + B_2 x_2 = f_2 \\
&\qquad\vdots \\
&-\widehat{B}_{j-1} x_{j-1} + B_j x_j = f_j \\
&\qquad\vdots \\
&-\widehat{B}_{N_T-1} x_{N_T-1} + B_{N_T} x_{N_T} = f_{N_T}.
\end{aligned} \tag{11}$$

In order to calculate the derivative of certain fit-do-data functionals in later sections, we will want to determine certain adjoint systems. For this purpose it is useful to rewrite these equations as a system

$$\begin{bmatrix} B_1 & 0 & \cdot & \cdot & \cdot & 0 \\ -\widehat{B}_1 & B_2 & 0 & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & 0 & -\widehat{B}_{N_T-1} & B_{N_T} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_{N_T} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ \cdot \\ \cdot \\ \cdot \\ f_{N_T} \end{bmatrix} + \begin{bmatrix} \widehat{B}_0 x_0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix} \tag{12}$$

or setting

$$\widehat{x} = \begin{bmatrix} x_0 \\ x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_{N_T} \end{bmatrix} \quad \text{and} \quad \widehat{f} = \begin{bmatrix} f_1 \\ f_2 \\ \cdot \\ \cdot \\ \cdot \\ f_{N_T} \end{bmatrix}$$

we have

$$\begin{bmatrix} B_1 & 0 & \cdot & \cdot & \cdot & 0 \\ -\widehat{B}_1 & B_2 & 0 & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & 0 & -\widehat{B}_{N_T-1} & B_{N_T} \end{bmatrix} \widehat{x} = \widehat{f} + \begin{bmatrix} \widehat{B}_0 x_0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}. \tag{13}$$

3. Data and formulation of the estimation problem

Data for the problem is in the form of the observed carbon flux for the region. In [2] the flux is expressed as a convolution of the carbon pool sizes. In this work it is useful to express the flux in terms of a product of vectors. To define the observable system output, we define the observation operator that maps the state, $x(c)$, of the differential equation associated with a parameter vector c.

Let

$$F_1 = 0.015, \quad F_2 = 0.0015, \quad F_3 = 0.015.$$

Introduce the matrix $\widehat{C}(t) = \tau(t)C$ and the column m-vector valued function $\widehat{c}(t) = \tau(t)c$. Further, define the constant valued column m-vectors.

$$e = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \quad \text{and} \quad f = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

and the $m \times m$ constant matrices

$$\widehat{I} = \begin{bmatrix} 0 & & & \cdot & \cdot & \cdot & & 0 \\ & 0 & & & & & & \\ & & 0 & & & & & \cdot \\ \cdot & & & 1 & 0 & & & \cdot \\ \cdot & & & 0 & \cdot & \cdot & & \cdot \\ \cdot & & & & \cdot & \cdot & \cdot & \\ & & & & & \cdot & \cdot & 0 \\ 0 & & & \cdot & \cdot & \cdot & 0 & 1 \end{bmatrix},$$

$$H = \begin{bmatrix} 0 & & & \cdot & \cdot & \cdot & & 0 \\ & \frac{1}{2} & & & & & & \\ & & 1 & & & & & \cdot \\ \cdot & & & 1 & 0 & & & \cdot \\ \cdot & & & 0 & \cdot & \cdot & & \cdot \\ \cdot & & & & \cdot & \cdot & \cdot & \\ & & & & & \cdot & \cdot & 0 \\ 0 & & & \cdot & \cdot & \cdot & 0 & 1 \end{bmatrix}.$$

We note that $\widehat{I}(H) = \widehat{I}$. Finally, we define the column m-vector valued function

$$\phi(c)(t) = H\{f + \widehat{c}(t) - \widehat{I}\widehat{C}(t)[I + A_0^{\mathrm{T}}]e\}. \tag{14}$$

The flux at time t corresponding to the vector of parameters c is defined to be

$$q(c)(t) = [\phi(c)(t)]^{\mathrm{T}} x(c)(t) \tag{15}$$

and denote the flux at time t_i by

$$q_i(c) = q(c)(t_i).$$

We denote the observed CO_2 flux by means of the vector $q^{\mathrm{o}} = \{q_i^{\mathrm{o}}\}_{i=1}^{N_0}$ representing measurements at times $\{t_i^{\mathrm{o}}\}_{i=1}^{N_0}$. To compare the flux associated with the parameter $cq(c)$ with the measurements q^{o}, we define the functional defined on the R^m by

$$J(c) = \frac{1}{2}\sum_{i=1}^{N_0}(q(c)(t_i^{\mathrm{o}}) - q_i^{\mathrm{o}})^2. \tag{16}$$

Our purpose now is to minimize the functional $J(c)$ over a set of admissible parameters $Q_{\mathrm{ad}} \subset R^m$ in order to determine the value of the parameter c that gives, within the context of our model, the best fit to the observed data q^{o}. Towards this end, we consider the problem

$$\text{Find } c_{\mathrm{opt}} \in Q_{\mathrm{ad}} \text{ such that } J(c_{\mathrm{opt}}) = \text{infimum } \{J(c) : c \in Q_{\mathrm{ad}}\}. \tag{17}$$

The existence of a solution to this minimization problem follows from the continuous dependence of the functional $J(\cdot)$ on c and properties such as the compactness of Q_{ad}.

4. Determination of the gradient of the fit-to-data functional

Our approach in this work is to use a descent minimization method. This requires the calculation of the derivative of $J(c)$ with respect to c. To facilitate the calculation, we introduce some notation.

Let $\Phi(c)$ denote the $N_0 \times (mN_0)$ matrix

$$\Phi(c) = \begin{bmatrix} \phi(c)(t_1^{\mathrm{o}})^{\mathrm{T}} & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & \phi(c)(t_2^{\mathrm{o}})^{\mathrm{T}} & & & & \cdot \\ \cdot & 0 & \cdot & & & \cdot \\ \cdot & & & \cdot & & \cdot \\ \cdot & & & & \cdot & 0 \\ 0 & \cdot & \cdot & \cdot & 0 & \phi(c)(t_{N_0}^{\mathrm{o}})^{\mathrm{T}} \end{bmatrix}$$

and let P denote the $(mN_0) \times (mN_T)$ matrix that projects the vector $\widehat{x}$ onto the space consisting of vectors x that are evaluated at observation times $\{t_i^{\mathrm{o}}\}_{i=1}^{N_0}$. Finally, define the vector of observations

$$\widehat{q}^{\mathrm{o}} = \begin{bmatrix} q_1^{\mathrm{o}} \\ \vdots \\ q_{N_0}^{\mathrm{o}} \end{bmatrix}.$$

We can rewrite the fit-to-data functional $J(c)$ in the form

$$J(c) = \frac{1}{2}(\Phi(c)P\widehat{x}(c) - \widehat{q}^{\mathrm{o}})^{\mathrm{T}}(\Phi(c)P\widehat{x}(c) - \widehat{q}^{\mathrm{o}}). \tag{18}$$

The derivative of the functional $J(c)$ is given by

$$DJ(c)c' = (\Phi(c)P\widehat{x}(c) - \widehat{q}^{\mathrm{o}})^{\mathrm{T}}([D\Phi(c)c']P\widehat{x}(c) + \Phi(c)P[Dx(c)c']). \tag{19}$$

For the term

$$(\Phi(c)P\widehat{x}(c) - \widehat{q}^{\mathrm{o}})^{\mathrm{T}}([D\Phi(c)c']P\widehat{x}(c),$$

we note that

$$[D\Phi(c)c']P\widehat{x}(c) = \begin{bmatrix} \tau(t_1)\{x(c)(t_1)^{\mathrm{T}}\widehat{I} - e^{\mathrm{T}}(I + A_0)\widehat{I}\ \operatorname{diag}\ (x(c)(t_1))\}c' \\ \vdots \\ \tau(t_{N_0})\{x(c)(t_{N_0})^{\mathrm{T}}\widehat{I} - e^{\mathrm{T}}(I + A_0)\widehat{I}\ \operatorname{diag}\ (x(c)(t_{N_0}))\}c' \end{bmatrix}.$$

We next calculate

$$(\Phi(c)P\widehat{x}(c) - \widehat{q}^{\mathrm{o}})^{\mathrm{T}}\Phi(c)P[Dx(c)c'].$$

To facilitate this calculation, we introduce the adjoint equations for the problem.

Referring to Eq. (13), the derivative of $\widehat{x}(c)$ with respect to c satisfies the set of equations

$$\begin{bmatrix} B_1(c) & 0 & \cdot & \cdot & \cdot & 0 \\ -\widehat{B}_1(c) & B_2(c) & 0 & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & 0 & -\widehat{B}_{N_T-1}(c) & B_{N_T}(c) \end{bmatrix} [D\widehat{x}(c)c']$$

$$= \begin{bmatrix} [D\widehat{B}_0(c)c']x_0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$- \begin{bmatrix} [DB_1(c)c'] & & & & \\ -[D\widehat{B}_1(c)c'] & [DB_2(c)c'] & & & \\ & \cdot & \cdot & & \\ & & \cdot & \cdot & \\ & & & \cdot & \cdot \\ & & & -[D\widehat{B}_{N_T-1}(c)c'] & [DB_{N_T}(c)c'] \end{bmatrix} \widehat{x}(c). \tag{20}$$

From Eq. (8) we obtain

$$B_j(c) = I - \theta \mathrm{d}t\tau(t_j)A_0 \operatorname{diag}(c)$$

so that

$$[DB_j(c)c']x = -\theta \mathrm{d}t\tau(t_j)A_0 \operatorname{diag}(x)c'. \tag{21}$$

From Eq. (9) it follows that

$$\widehat{B}_j(c) = I + (1-\theta)\mathrm{d}t\tau(t_j)A_0 \operatorname{diag}(c)$$

and we have similarly

$$[D\widehat{B}_j(c)c']x = (1-\theta)\mathrm{d}t\tau(t_j)A_0 \operatorname{diag}(x)c'. \tag{22}$$

It follows from Eq. (20) that

$$\begin{bmatrix} B_1(c) & 0 & \cdot & \cdot & \cdot & 0 \\ -\widehat{B}_1(c) & B_2(c) & 0 & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & 0 & -\widehat{B}_{N_T^{-1}}(c) & B_{N_T}(c) \end{bmatrix} [D\widehat{x}(c)c']$$

$$= \begin{bmatrix} [D\widehat{B}_0(c)c']x_0 - [DB_1(c)c']x_1(c) \\ [D\widehat{B}_1(c)c']x_1(c) - [DB_2(c)c']x_2(c) \\ \vdots \\ [D\widehat{B}_{N_T^{-1}}(c)c']x_{N_T^{-1}}(c) - [DB_{N_T}(c)c']x_{N_T}(c) \end{bmatrix}$$

and using Eqs. (21) and (22) we find

$$\begin{bmatrix} B_1(c) & 0 & \cdot & \cdot & \cdot & 0 \\ -\widehat{B}_1(c) & B_2(c) & 0 & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & 0 & -\widehat{B}_{N_T-1}(c) & B_{N_T}(c) \end{bmatrix} [D\widehat{x}(c)c']$$

$$= \begin{bmatrix} [(1-\theta)\mathrm{d}t\tau(t_0)A_0 \ \mathrm{diag}(x_0) + \theta\mathrm{d}t\tau(t_1)A_0 \ \mathrm{diag}(x_1(c))]c' \\ [(1-\theta)\mathrm{d}t\tau(t_1)A_0 \ \mathrm{diag}(x_1(c)) + \theta\mathrm{d}t\tau(t_2)A_0 \ \mathrm{diag}(x_2(c))]c' \\ \vdots \\ [(1-\theta)\mathrm{d}t\tau(t_{N_{T-1}})A_0 \ \mathrm{diag}(x_{N_{T-1}}(c)) + \theta\mathrm{d}t\tau(t_{N_T})A_0 \ \mathrm{diag}(x_{N_T}(c))]c' \end{bmatrix}.$$

Introduce the adjoint variable as the mN_T-column vector

$$\widehat{p} = \begin{bmatrix} p_1 \\ \vdots \\ P_{N_T} \end{bmatrix}$$

and form the products

$$\widehat{p}^{\mathrm{T}} \begin{bmatrix} B_1(c) & 0 & \cdot & \cdot & \cdot & 0 \\ -\widehat{B}_1(c) & B_2(c) & 0 & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & 0 & -\widehat{B}_{N_T-1}(c) & B_{N_T}(c) \end{bmatrix} [D\widehat{x}(c)c']$$

$$= \widehat{p}^{\mathrm{T}} \begin{bmatrix} [(1-\theta)\mathrm{d}t\tau(t_0)A_0 \ \mathrm{diag}(x_0) + \theta\mathrm{d}t\tau(t_1)A_0 \ \mathrm{diag}(x_1(c))]c' \\ [(1-\theta)\mathrm{d}t\tau(t_1)A_0 \ \mathrm{diag}(x_1(c)) + \theta\mathrm{d}t\tau(t_2)A_0 \ \mathrm{diag}(x_2(c))]c' \\ \vdots \\ [(1-\theta)\mathrm{d}t\tau(t_{N_{T}-1})A_0 \ \mathrm{diag}(x_{N_{T}-1}(c)) + \theta\mathrm{d}t\tau(t_{N_T})A_0 \ \mathrm{diag}(x_{N_T}(c))]c' \end{bmatrix}.$$

to obtain

$$\begin{aligned} &\widehat{p}^{\mathrm{T}} \begin{bmatrix} B_1(c) & 0 & \cdot & \cdot & \cdot & 0 \\ -\widehat{B}_1(c) & B_2(c) & 0 & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & 0 & -\widehat{B}_{N_T-1}(c) & B_{N_T}(c) \end{bmatrix} [D\widehat{x}(c)c'] \\ &\quad = \{p_1^{\mathrm{T}}[(1-\theta)\mathrm{d}t\tau(t_0)A_0 \ \mathrm{diag}(x_0) + \theta\mathrm{d}t\tau(t_1)A_0 \ \mathrm{diag}(x_1(c))] + \cdots \\ &\qquad + p_{N_T}^{\mathrm{T}}[(1-\theta)\mathrm{d}t\tau(t_{N_T}-1)A_0 \ \mathrm{diag}(x_{N_t-1}) \\ &\qquad + \theta\mathrm{d}t\tau(t_{N_t})A_0 \ \mathrm{diag}(x_{N_T}(c))]\}c'. \end{aligned}$$

Now set

$$\begin{aligned} &\widehat{p}^{\mathrm{T}} \begin{bmatrix} B_1(c) & 0 & . & . & . & 0 \\ -\widehat{B}_1(c) & B_2(c) & 0 & . & . & . \\ 0 & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & 0 \\ 0 & . & . & 0 & -\widehat{B}_{N_T-1}(c) & B_{N_T}(c) \end{bmatrix} \\ &\quad = [\Phi(c)P\widehat{x}(c) - \widehat{q}^{\mathrm{o}}]^{\mathrm{T}}\Phi(c)P. \end{aligned}$$

or taking the transpose of both sides

$$\begin{aligned} &\begin{bmatrix} B_1(c)^{\mathrm{T}} & -\underset{1}{\widehat{B}}(c)^{\mathrm{T}} & . & . & . & 0 \\ 0 & \widehat{B}_2(c)^{\mathrm{T}} & 0 & . & . & . \\ 0 & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & -\widehat{B}_{N_T-1}(c)^{\mathrm{T}} \\ 0 & . & . & 0 & 0 & B_{N_T}(c)^{\mathrm{T}} \end{bmatrix} \widehat{p}(c) \\ &\quad = P^{\mathrm{T}}\Phi(c)^{\mathrm{T}}\Phi(c)P\widehat{x}(c) - P^{\mathrm{T}}\Phi(c)^{\mathrm{T}}\widehat{q}^{\mathrm{o}}, \end{aligned}$$

The vector on the right is given by

$$P^{\mathrm{T}}\Phi(c)^{\mathrm{T}}\Phi(c)P\widehat{x}(c) - P^{\mathrm{T}}\Phi(c)^{\mathrm{T}}\widehat{q}^{\mathrm{o}} = \begin{bmatrix} g_1 \\ g_2 \\ 0 \\ 0 \\ 0 \\ g_{N_T} \end{bmatrix}$$

where $g_i = 0$ unless the subscript i corresponds to the subscript of an observation time t_i^{o} in which case

$$g_i = \phi(c)(t_i^{\mathrm{o}})^{\mathrm{T}}(\phi(c)(t_i^{\mathrm{o}})x(c)(t_i^{\mathrm{o}}) - x(c)(t_i^{\mathrm{o}})).$$

The adjoint system is solved in the reverse order of the forward equation. Thus, we solve the system

$$\begin{aligned} &B_{N_T}(c)^{\mathrm{T}}p_{N_T}(c) = g_{N_T} \\ &B_{N_T-1}(c)^{\mathrm{T}}p_{N_T-1}(c) - \widehat{B}_{N_T}(c)^{\mathrm{T}}p_{N_T}(c) = g_{N_T-1} \\ &\qquad\qquad\vdots \\ &B_1(c)^{\mathrm{T}}p_1(c) - \widehat{B}_1(c)^{\mathrm{T}}p_2(c) = g_1. \end{aligned}$$

Combining the terms we find the derivative of J to satisfy

$$\begin{aligned} DJ(c)c' = {} & \{p_1^{\mathrm{T}}[(1-\theta)\mathrm{d}t\tau(t_0)A_0 \ \mathrm{diag}(x_0) + \theta\mathrm{d}t\tau(t_1)A_0 \ \mathrm{diag}(x_1(c))] + \cdots \\ & + p_{N_T}^{\mathrm{T}}[(1-\theta)\mathrm{d}t\tau(t_{N_T-1})A_0 \ \mathrm{diag}(x_{N_T-1}(c)) \\ & + \theta\mathrm{d}t\tau(t_{N_T})A_0 \ \mathrm{diag}(x_{N_T}(c))]\}c' \\ & + \{[\phi_1(c)^{\mathrm{T}}x(c)(t_1^{\mathrm{o}}) - q_1^{\mathrm{o}}]\tau(t_1^{\mathrm{o}})[(x(c)(t_1^{\mathrm{o}})^{\mathrm{T}}\widehat{I} \\ & - e^{\mathrm{T}}(I+A_0)\widehat{I} \ \mathrm{diag}(x(c)(t_1^{\mathrm{o}}))] + \cdots + \{[\phi_{N_0}(c)^{\mathrm{T}}x(c)(t_{N_0}^{\mathrm{o}}) - q_{N_0}^{\mathrm{o}}] \\ & \times \tau(t_{N_0}^{\mathrm{o}})[(x(c)(t_{N_0}^{\mathrm{o}})^{\mathrm{T}}\widehat{I} - \ e^{\mathrm{T}}(I+A_0)\widehat{I} \ \mathrm{diag}(x(c)(t_{N_0}^{\mathrm{o}}))]\}c'. \qquad (23) \end{aligned}$$

From Eq. (23) we see that the $DJ(c)$ is the gradient of the functional $J(c)$ and is given by the column m-vector

$$\begin{aligned} DJ(c) = {} & \{p_1^{\mathrm{T}}[(1-\theta)\mathrm{d}t\tau(t_0)A_0 \, \mathrm{diag}(x_0) + \theta\mathrm{d}t\tau(t_1)A_0 \, \mathrm{diag}(x_1(c))] + \cdots \\ & + p_{N_T}^{\mathrm{T}}[(1-\theta)\mathrm{d}t\tau(t_{N_T-1})A_0 \, \mathrm{diag}(x_{N_T-1}(c)) \\ & + \theta\mathrm{d}t\tau(t_{N_T})A_0 \, \mathrm{diag}(x_{N_T}(c))] + [\phi_1(c)^{\mathrm{T}}x(c)(t_1^{\mathrm{o}}) - q_1^{\mathrm{o}}]\tau(t_1^{\mathrm{o}})[(x(c)(t_1^{\mathrm{o}})^{\mathrm{T}}\widehat{I} \\ & - e^{\mathrm{T}}(I+A_0)\widehat{I} \, \mathrm{diag}(x(c)(t_1^{\mathrm{o}}))] + \cdots + [\phi_{N_0}(c)^{\mathrm{T}}x(c)(t_{N_0}^{\mathrm{o}}) - q_{N_0}^{\mathrm{o}}] \\ & \times \tau(t_{N_0}^{\mathrm{o}})[(x(c)(t_{N_0}^{\mathrm{o}})^{\mathrm{T}}\widehat{I} - e^{\mathrm{T}}(I+A_0)\widehat{I} \, \mathrm{diag}(x(c)(t_{N_0}^{\mathrm{o}}))]\}^{\mathrm{T}}. \qquad (24) \end{aligned}$$

Eq. (24) gives a computably efficient expression for $DJ(c)$ that will be used in minimization algorithms of the following section.

5. Testing against the duke forest data

We consider two data sets that give CO_2 flux observations from the Duke Forest for ambient and elevated carbon influx functions $u(t)$. Figs. 1 and 2 graphically show measurements of the influx functions $u(t)$ for the two experiments. The temperature and moisture functions whose product determines the function $\tau(t)$ are shown in Figs. 3 and 4, respectively. Even though the inputs shown in Figs. 1–4 apparently have considerable noise, smoothed versions of the data may be used. However, the noise in the inputs indicated seems to have little effect on the solution.

We consider an iterative local minimization method to approximate a minimizer of the functional J even though there may in fact be multiple minima. We will address this possibility later. We indicate the minimization procedure.

(i) Starting from and initial guess c_0 that is physically reasonable, the derivative $DJ(c_0)$, column m-vector, of the functional J is calculated at the point c_0. The derivative is calculated by introducing the adjoint as indicated in the previous section.
(ii) From the derivative a descent direction $d(c_0)$ may be determined. For example, in the steepest descent method

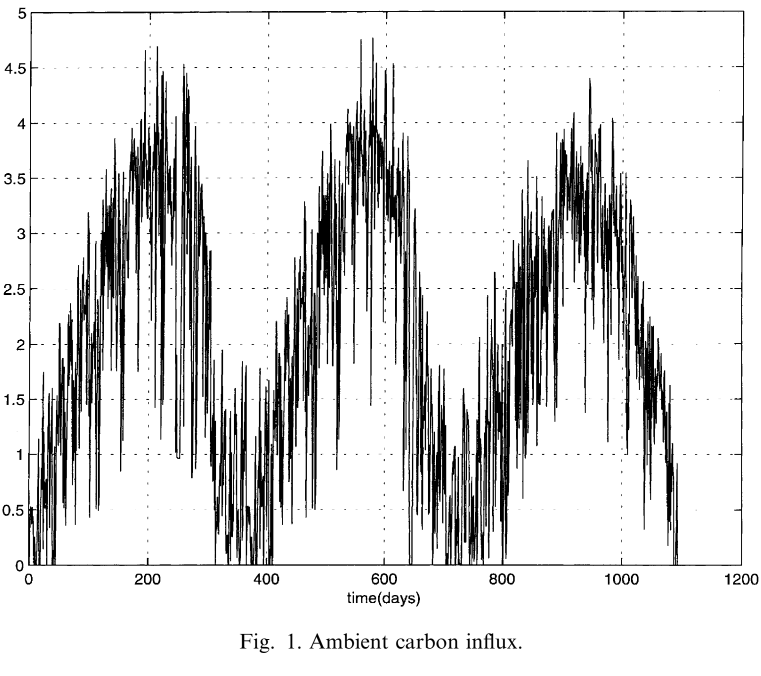

Fig. 1. Ambient carbon influx.

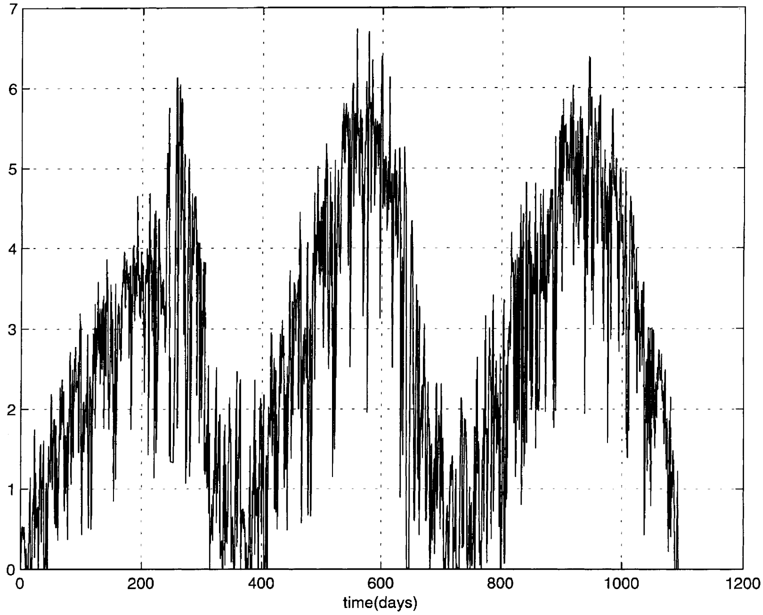

Fig. 2. Elevated carbon influx.

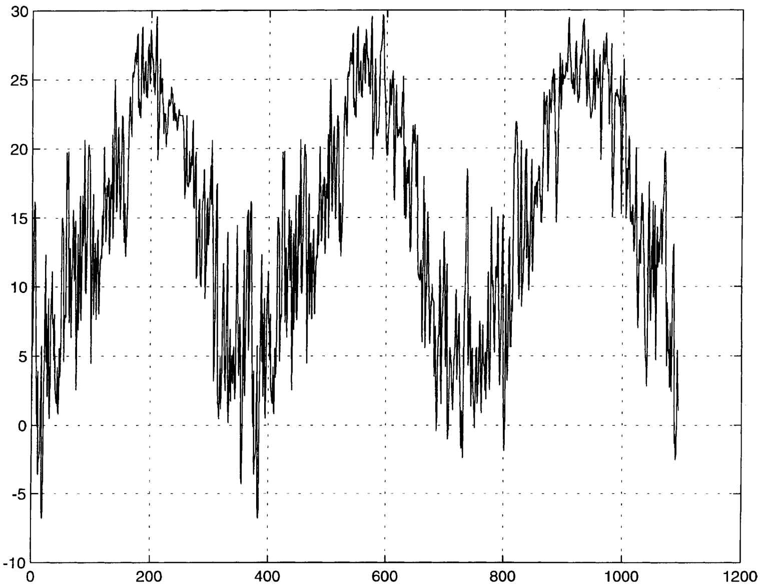

Fig. 3. Temperature function.

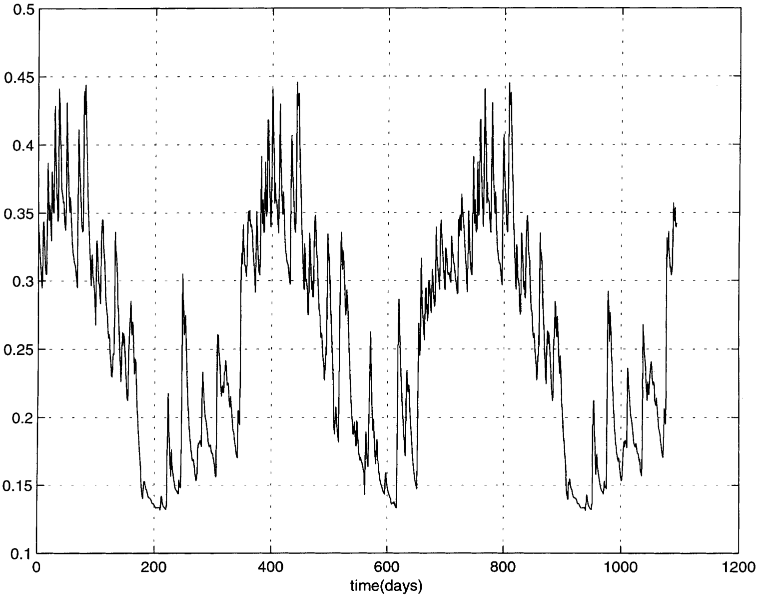

Fig. 4. Moisture function.

$$d(c_0) = \frac{-DJ(c_0)}{\|DJ(c_0)\|}.$$

Other more effective methods are obtained by choosing the descent direction differently. However, such methods usually involve computation of the derivative as some level.

(iii) A search is then conducted along the direction by generating parameter points

$$c_1^k = c_0 + \varepsilon_k d(c_0),$$

where for each $k = 1, \ldots, L, \varepsilon_k$ is a real number and decreases as k increases. For example, set $\varepsilon_k = 1/2^k$ for $k = 1, \ldots, 5$.

(iv) Evaluate the functional J at each such parameter vector. This step requires repeatedly solving the forward problem in order to evaluate the functional. The updated parameter vector c_1 is selected to be the first c_1^k such that

$$J(c_1^k) < J(c_0).$$

(v) The procedure continues by replacing c_0 by c_1 above and repeating the above steps.

For our computations we use two sets of data. In each case we seek to estimate the parameter vector c. In both cases the parameter vector c is initialized to be where

$$c_0 = \begin{bmatrix} 2.65 \times 10^{-3} \\ 1.89 \times 10^{-4} \\ 3.94 \times 10^{-3} \\ 1.75 \times 10^{-3} \\ 1.07 \times 10^{-2} \\ 5.42 \times 10^{-3} \\ 9.04 \times 10^{-3} \\ 2.15 \times 10^{-3} \\ 4.67 \times 10^{-2} \\ 5.64 \times 10^{-3} \\ 2.29 \times 10^{-4} \\ 9.83 \times 10^{-6} \end{bmatrix}.$$

In Figs. 5 and 7 we show the performance of the value of the functional as a function of the iteration for the ambient and the elevated data sets, respectively. Note that after the first couple of iterations the value of the criterion is basically unchanged. The comparison of the calculated output to the data in each case is presented in Figs. 6 and 8.

The R^2 of the initial value is 0.81. While the minimization of the functional does not take into account R^2, the value is monitored and in fact increases to approximately 0.85 for both cases. The estimated transfer coefficient vectors are

$$c_{e1} = \begin{bmatrix} 2.64 \times 10^{-3} \\ 0 \\ 3.94 \times 10^{-3} \\ 1.75 \times 10^{-3} \\ 1.07 \times 10^{-2} \\ 5.43 \times 10^{-3} \\ 9.04 \times 10^{-3} \\ 2.16 \times 10^{-3} \\ 4.68 \times 10^{-3} \\ 5.65 \times 10^{-3} \\ 1.27 \times 10^{-4} \\ 0 \end{bmatrix}$$

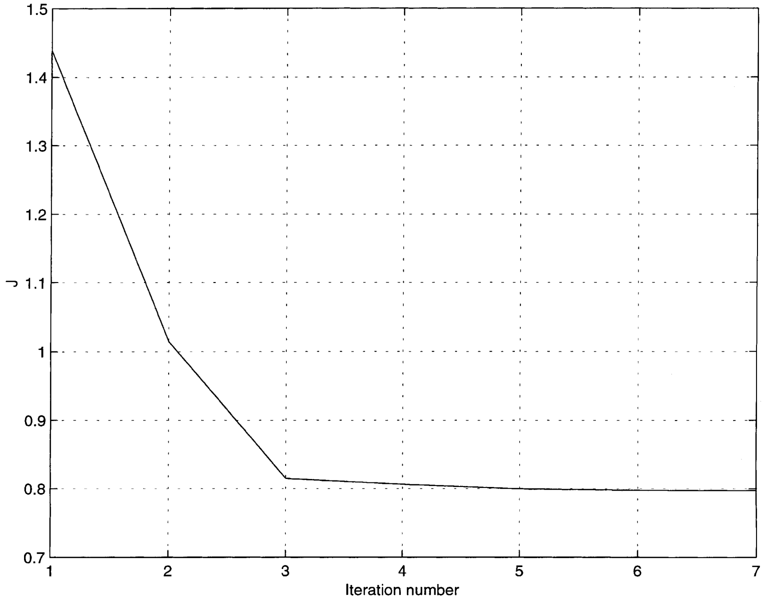

Fig. 5. Value of the criterion J during descent for the ambient data case.

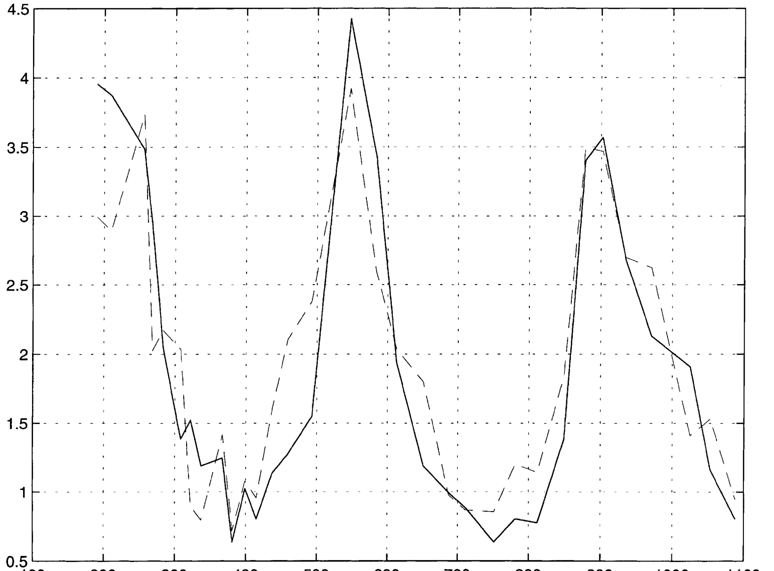

Fig. 6. Comparison of model output flux (dashed) with data (solid) ambient case.

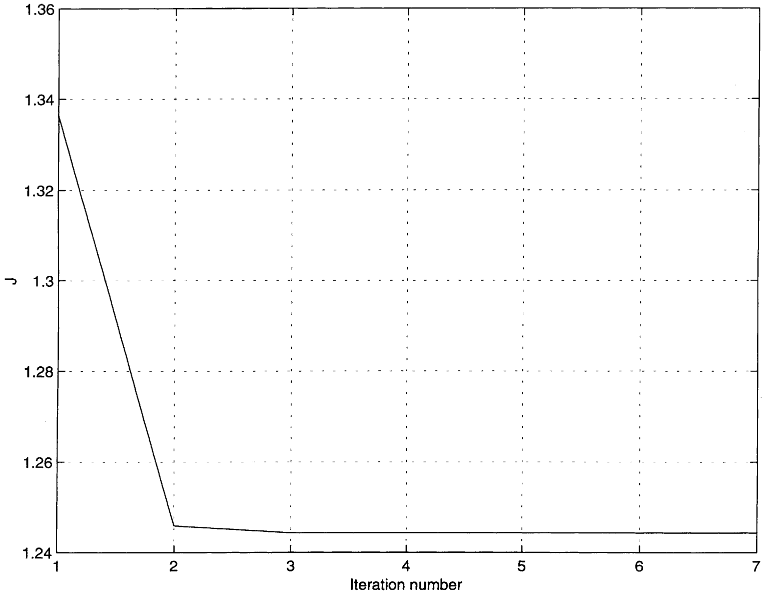

Fig. 7. Value of the criterion J during descent for the elevated data case.

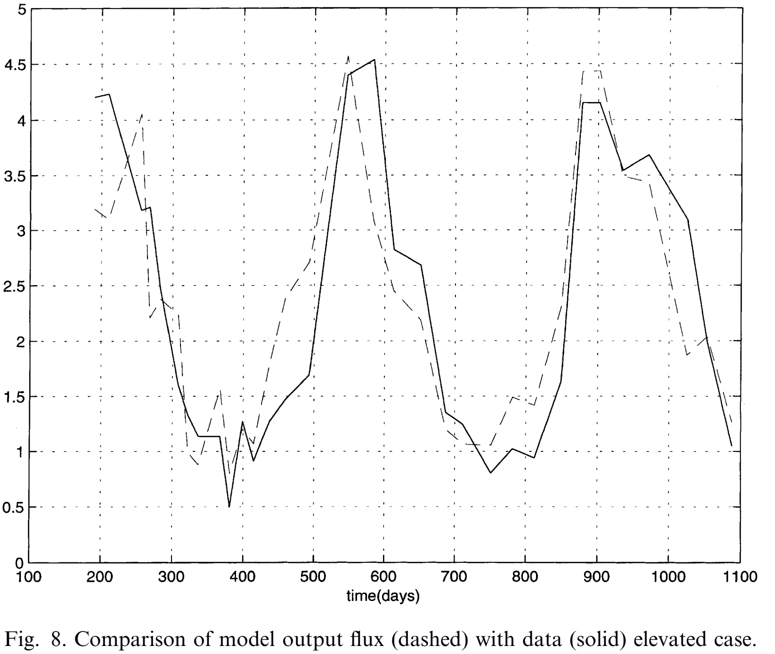

Fig. 8. Comparison of model output flux (dashed) with data (solid) elevated case.

and

$$c_{e2} = \begin{bmatrix} 2.66 \times 10^{-3} \\ 1.41 \times 10^{-4} \\ 3.94 \times 10^{-3} \\ 1.75 \times 10^{-3} \\ 1.07 \times 10^{-2} \\ 5.42 \times 10^{-3} \\ 9.04 \times 10^{-3} \\ 2.15 \times 10^{-3} \\ 4.67 \times 10^{-3} \\ 5.64 \times 10^{-3} \\ 1.91 \times 10^{-4} \\ 3.55 \times 10^{-7} \end{bmatrix}$$

for the ambient and elevated data, respectively. The relative effect between the two CO_2 treatments on the estimated transfer vectors is given by

$$\text{Relative effect} = \frac{\|c_{e2} - c_{e1}\|}{\|c_{e1}\|} = 3.67 \times 10^{-3}$$

or a relative effect to less than 0.4%.

6. Significance of the results

The carbon transfer coefficient vector c ecologically defines the efficiency of carbon delivering to and storage in various plant and soil carbon pools. The ensemble of all the transfer coefficients represents the capacity of an ecosystem to retain carbon in plant and soil. Comparison of the rates at elevated CO_2 with those at ambient CO_2 is an indication of whether the capacity of terrestrial carbon sequestration is sustained as the atmospheric CO_2 concentration is increasing. In our study at the Duke FACE, the estimated transfer coefficients at elevated CO_2 are well correlated with those at ambient CO_2, expect for that from the passive soil carbon pool. The relative variation between the two estimated transfer vectors is less than 0.4%. The virtually identical transfer coefficients indicate that the potential of the Duke Forest to sequester carbon is hardly affected by rising atmospheric CO_2. Therefore, up-to-date experimental results from the FACE experiment suggest a sustainable carbon sink in the Duke Forest.

The estimation of the carbon transfer coefficients is primarily based on soil surface respiration observed at the Duke FACE project. While the observed soil respiration is a good data set to reflect system-level behavior of terrestrial ecosystem, the estimates of the carbon transfer coefficients can be future improved by incorporation of other data sets into the model-data comparison.

Acknowledgements

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