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Climatic information from $\delta^{13}C$ in plants by combining statistical and mechanistic approaches

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Abstract: The approach commonly used to assess the potential for climate reconstruction is to use linear regressions to compare the isotopic signal stored in archives to instrumental climatic data sets. A new method is proposed that combines statistical and mechanistic approaches to extract climatic information from $\delta^{13}C$ records in organic matter. Both a spatial and a temporal gradient of ^{13}C discrimination in a moss species commonly found in temperate and tropical peat bogs are compared to meteorological records. The relevance of fossil and modern analogues to elucidate palaeoenvironment records are tested. It was found that the magnitude and, in some cases, the direction of the impact of temperature, humidity and CO_2 atmospheric concentration on ^{13}C discrimination depend on the calibration set considered. The use of a mechanistic model is shown to help greatly in specifying the joint influence of the climatic variables.

Key words: Carbon isotopes, plant organic matter, *Sphagnum* species, modern analogue, climate reconstruction, statistical and mechanistic approaches.

Introduction

Plant organic material stored in continental archives such as peat bogs or tree rings offers the possibility to reconstruct past climatic conditions on timescales ranging from annual to millennial (Aucour *et al.*, 1999; Hong *et al.*, 2000; Pendall *et al.*, 2001; White *et al.*, 1994a). However, its potential for climate reconstruction can only be realized if measurable parameters within the accumulated organic matter, such as stable isotopes, can be interpreted in terms of one or more climatic variables. The approach commonly used to resolve and quantify the influence of climate on isotopic records is to empirically calibrate the variation in isotopes to known climatic variation using meteorological records. Typically, this is done by performing linear regressions comparing one or more isotopes and various climate parameters (Anderson *et al.*, 2002; Fauquette *et al.*, 1998; Wilf *et al.*, 1998). For example, this approach has been used to resolve the influence of precipitation, temperature and atmospheric CO_2 concentration on carbon isotopic composition ($\delta^{13}C$) variations in trees (Anderson *et al.*, 1998; Edwards *et al.*, 2000; Lipp *et al.*, 1996; Robertson *et al.*, 2001; Saurer and Siegenthaler, 1995).

A second approach for interpreting plant isotopic variation in terms of climate is to try to understand the underlying causes of isotopic fractionation in plants. Laboratory and field studies have led to the development of mechanistic models that link isotopic variations in plants to specific physical or biological fractionation mechanisms. In a few cases, these relationships were used to reconstruct past climatic variations. For instance, at a few locations only one climatic variable is the limiting factor and thus controls the isotopic fractionation (as precipitation in desert area; Lipp *et al.*, 1996), or when plant species for which a mechanistic model is relatively well constrained are considered (Aucour *et al.*, 1996; Edwards *et al.*, 1985; Pendall *et al.*, 2001). However, for the majority of plant species, mechanistic models are not well constrained. This is the case for one of the ubiquitous species of bog plants, *Sphagnum magellanicum*.

In this study we investigate how the $\delta^{13}C$ values of cellulose from one species of moss, *Sphagnum magellanicum*, responds to spatial and temporal changes in climate. We propose a new approach to derive transfer functions between $\delta^{13}C$ in plants and temperature, humidity and CO_2 concentration. Furthermore, because it is often assumed that plant-climate relationships are interchangeable between spatial and temporal calibrations, we compare the validity of these two approaches. One of the main issues addressed in this study is to test the

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relevance of fossil and modern analogues to elucidate palaeoenvironment records.

Definitions and notations

The difference between the stable carbon isotopic composition of a plant and its carbon source (the atmospheric CO_2) is called the discrimination (Δ). Δ is related to the ratio of ambient ($[CO_2]_a$) to intracellular ($[CO_2]_i$) CO_2 concentrations by the simple model developed for C_3 plants (equation (1); Farquhar *et al.*, 1982):

$$\Delta = \delta^{13}C_{atm} - \delta^{13}C_{plant} = a + (b - a)\left(\frac{[CO_2]_i}{[CO_2]_a}\right) \qquad (1)$$

where the constant a is the fractionation factor associated with the different diffusivities of $^{12}CO_2$ and $^{13}CO_2$ and the constant b is the fractionation induced by carbon fixation at carboxylation sites. The CO_2 concentration gradient between the cellular space and ambient air depends on the plant assimilation rate and on the resistance to CO_2 diffusion through the cell walls (von Caemmerer and Evans, 1991).

Similar models were developed for nonvascular plants such as mosses. Laboratory studies (Proctor, 1982; Proctor *et al.*, 1992; Rice and Giles, 1996) and field studies (Murray *et al.*, 1989; Price *et al.*, 1997; Silvola, 1985) investigated moss responses to changes in different climate parameters (such as temperature, humidity and $[CO_2]_a$). More precisely, the climatic control on moss isotopic discrimination is exerted through the assimilation rate; its analytical expression is given by Figge and White (1995):

$$\Delta = a + (b - a) \times \left(1 - \frac{r \times P^0_{max}(1 + \lambda(T - T_0)) \times (\alpha + \beta[CO_2]_a) \times \frac{W(h) - W_{dry}}{W_{opt} - W_{dry}}}{[CO_2]_a}\right) \qquad (2)$$

In equation (2), P^o_{max} is the maximum assimilation rate for modern conditions ($T_0 = 7°C$), $T - T_0$ is the assumed temperature variation in the past, scaled by an adaptation factor, λ (White *et al.*, 1994b). W(h) is the moss water content in the moss cell that directly depends on ambient air humidity, h, W_{dry} and W_{opt} are the dry and optimum water content, respectively, and α and β are species-specific constants. Equation (2) summarizes the mechanistic model that guides the present study.

Methods

Sample collection and preparation

We took two approaches to investigate the carbon isotopic response of one of the most common species of peat-bog plants, *Sphagnum magellanicum*, to changing climatic conditions. First, samples of *S. magellanicum* were collected from a suite of 12 raised bogs in 1997 along an altitude transect between 500 and 2000 m high in the Bernese Alps, Switzerland (Figure 1). Compared to temporal variations, the altitude transect covers a wide range of climatic conditions in terms of temperature, $[CO_2]_a$ and humidity (Table 1). Secondly, we compared isotopic variation of hand-picked *S. magellanicum* from a well-dated core to meteorological records covering the past ~200 years. The fossil samples were extracted from a peat core drilled at the Rötmoos bog in 1999 (Figure 1). The core was extracted using a Wardenaar peat profile sampler (Wardenaar, 1987) designed to remove a large undisturbed peat monolith from the surface layer of the bog. On return to the laboratory, the peat core was frozen and then sectioned into 1 cm slices. The moss fragments of every second peat slice for the topmost 20 cm of the core, and every fourth slice deeper in the core, were removed and individual plant pieces were separated from the bulk peat under a binocular microscope. The individual pieces were then identified to the species level from these separates.

Both modern and fossil plant samples were freeze-dried and milled using a commercial modified coffee mill (Borella, 1998).

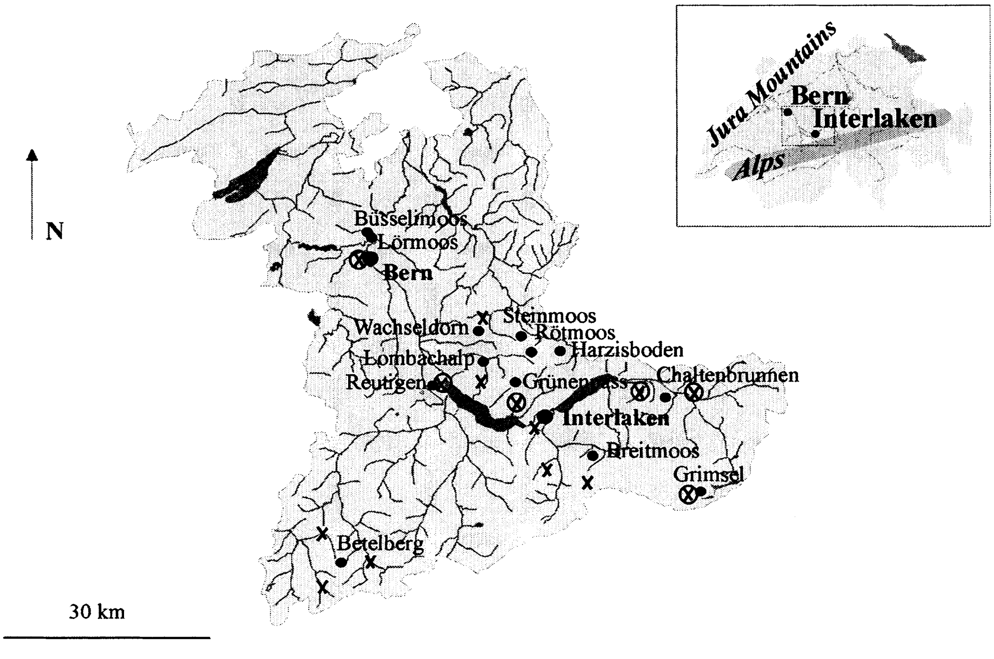

Figure 1 Location of the 12 study sites (closed circles) together with the meteorological stations from the Schweizerische Meteorologische Ansthalt (SMA) considered in this study (crosses). The inset shows the general location of the studied area in Switzerland.

Table 1 Climatic description of the sampling sites. The altitude, $[CO_2]_a$, temperature and relative humidity values correspond to mean monthly values during growing season (May to September)

Name of site	Altitude (m a.s.l.)	$[CO_2]_a$ (ppm)	Temp. (°C)	Relative humidity (%)
Lörmoos	583	313.6	16.7	72.8
Reutigen	620	314.0	15.9	72.8
Steinmoos	960	301.6	14.1	76.0
Wachseldorn	1000	300.9	13.7	76.0
Harzisboden	1100	296.3	12.8	74.6
Rötmoos	1200	292.9	12.3	76.6
Reutigen	1520	281.6	10.4	75.4
Grünenpass	1570	279.2	9.9	75.4
Breitmoos	1590	277.6	10.4	72.2
Chaltenbrunnen	1750	273.5	9.0	74.0
Betelberg	1800	266.9	8.9	74.0
Grimsel	1950	266.9	9.7	77.6

A subsample of the resulting powder was used for carbon isotope measurements of total plant carbon. A chemical extraction was performed on the remaining powder to obtain pure carbon α-cellulose (for more details, see (Ménot and Burns, 2001)). $\delta^{13}C$ values were determined by isotopic ratio mass spectrometry online continuous-flow method (EA-IRMS). A Carlo Erba 1500 Elementar Analyser was used for carbon isotopes as a combustion unit to generate CO_2. Gases were then driven by a helium stream through a gas chromatographic column to separate gas peaks. Isotopic ratios of CO_2 gases were then measured by a VG Prism II ratio mass spectrometer. Each sample was measured in triplicate. Ratios were reported relative to the Vienna Peedee belemnite international standard (VPDB). For a single set of analyses ($n = 100$, generally one day) the mean standard deviation for measurements of the graphite standard of the US National Bureau of Standards (NBS-21) and of an internal α-cellulose standard versus the reference gas value were 0.22‰ and 0.19‰, respectively.

A chronology of the core was developed using both ^{210}Pb and ^{14}C measurements. Twenty samples, taken every 2.5 cm from the top 50 cm of the core, were analysed by direct gamma assay for ^{210}Pb, ^{226}Ra, ^{137}Cs and ^{241}Am (Appleby *et al.*, 1986) at the Environmental Radioactivity Laboratory of Liverpool University. Age data were calculated using the Constant Rate of Supply (CRS) model (Appleby *et al.*, 1997). Three deep samples (at 60.5, 72.5 and 83.5 cm) were dated by ^{14}C decay counting at the Physic Institute of the University of Bern. Results, given first in conventional radiocarbon age dates, are converted into calibrated ^{14}C ages using the OxCal v.3.5 program (Bronk Ramsey, 2001).

Atmospheric $\delta^{13}C$ and meteorological data

For modern plants, isotopic discrimination is easily calculated by subtracting the measured cellulose $\delta^{13}C$ value from that of the modern atmosphere. In order to correctly estimate plant carbon isotopic discrimination in fossil plants, however, changes in the carbon isotopic composition of atmospheric CO_2 need to be taken into account. Direct measurements of atmospheric CO_2 are available for the last 150 years (Francey *et al.*, 1995; Keeling *et al.*, 1995). For earlier times, several records based on measurements in air bubbles in polar ice can be used (Francey *et al.*, 1995; 1998; Friedli *et al.*, 1986; Keeling *et al.*, 1995). To obtain a continuous record of $\delta^{13}C_{atm}$, stepwise linear function through the data of Friedli *et al.* (1986) and Francey *et al.* (1998) was used (Leuenberger *et al.*, personal communication).

The dense network of the Schweizerische Meteorologische Anstalt (SMA) weather stations near our study sites (Figure 1) provided a continuous tri-daily record of climatic variables such as temperature, relative humidity and atmospheric pressure at different altitudes. Some records from the SMA stations are continuous over the last 120 years.

Therefore, we obtained two data sets of Δ values and their corresponding meteorological environment. One consists of data collected along the altitude transect (spatial calibration set), and one consists of gathered over time from the core (temporal calibration set).

Traditional isotopic proxy methods

The standard approach to resolve the influence of climate on an isotopic data set from a climate archive is to calculate a transfer function using a simple or multiple linear regression of the measured climate proxy on meteorological variables (Edwards *et al.*, 1985; Lipp *et al.*, 1996). Applied to Δ, the relationship takes the following form:

$$\Delta = m_0 + m_1 h + m_2 T + m_3 [CO_2]_a \qquad (3)$$

where m_0, m_1, m_2, m_3 are parameters that are estimated, using the ordinary least square (OLS) econometric method (Davidson and McKinnon, 2004) . The transfer function is then rearranged to reconstruct climatic variable parameters. For example, if $[CO_2]_a$ is reconstructed, equation (4) is used:

$$[CO_2]_a = \frac{1}{m_3}(\Delta - m_0 - m_1 h - m_2 T) \qquad (4)$$

Model development: combining statistical and mechanistic approaches

We present a new approach, referred as the mechanistic approach, in which the information on plant physiology given by theoretical studies is taken into account to constrain the transfer function. Rewriting equation (2) yields:

$$\Delta = n_0 + n_1 \log(h) + n_2 \log(h)T + n_3 \frac{\log(h)}{[CO_2]_a} + n_4 \frac{\log(h)T}{[CO_2]_a} \qquad (5)$$

where the constants n_0, n_1, n_2, n_3 and n_4 are estimated and can be related to the model of Figge and White (1995) (see Note at end of article). The explanatory variables are combination of the climatic parameters in this analytical expression. Similar to the traditional transfer function approach, equation (5) is rearranged to predict the values of meteorological parameter. For instance, for $[CO_2]_a$, equation (5) becomes:

$$[CO_2]_a = \frac{(n_3 \log(h) + n_4 \log(h)T)}{(\Delta - n_0 - n_1 \log(h) - n_2 \log(h)T)} \qquad (6)$$

We further propose a second alternative, called the inverse mechanistic approach, in which the inverse form of the mechanistic transfer function (equation (6)) is directly estimated. Since equation (6) is nonlinear in the unknown parameters, in order to keep statistical methods simple, we approximate it by equation (7), which is estimated with the OLS procedure:

$$[CO_2]_a \approx N_0 + N_1T + N_2\frac{\log(h)}{b-\Delta} + N_3\frac{T\log(h)}{b-\Delta} + N_4\frac{b-\Delta}{\log(h)} \tag{7}$$

where N_0, N_1, N_2, N_3 and N_4 are the new parameters to be estimated. Similarly, temperature is expressed as a linear function of

$$\frac{1}{[CO_2]_a}, \frac{b-\Delta}{\log(h)}, \frac{b-\Delta}{\log(h)[CO_2]_a}, [CO_2]_a \text{ and } \frac{b-\Delta}{\log(h)}[CO_2]_a$$

Humidity is expressed as a linear function of

$$(b-\Delta)[CO_2]_a, \frac{b-\Delta}{T}, \frac{b-\Delta}{T}[CO_2]_a \text{ and } \frac{[CO_2]_a}{T}$$

The advantage of this method is that the transfer function used to reconstruct T, h and $[CO_2]_a$ is directly estimated and thus the errors associated with the estimations are minimized. The reconstructions of climatic variables are necessarily improved.

Using measured climate values for T, h, and $[CO_2]_a$, each of these three model approaches can be used to calculate a theoretical value of Δ for each peat bog site and for past temporal variation at the Rötmoos site. Comparing these calculated values to measured values will allow estimation of the utility of each approach.

Results

Trends in isotopic variations

The topmost 35 cm of the peat core collected at Rötmoos cover the last 70 years with a time resolution ranging from 1 to 5 years, the age-depth model being well constrained by ^{210}Pb analyses (Figure 2a). The temporal variations of $\delta^{13}C$ measured in α-cellulose and bulk material from *Sphagnum magellanicum* range between −22.1 and −25.3‰ (Figure 2b). Although there is somewhat less variability of α-cellulose $\delta^{13}C$ values, both α-cellulose and bulk material values exhibit similar trends. Values centred around −23.4 ± 0.4‰ and −23.0 ± 0.5‰ for bulk plant material and α-cellulose values, respectively, between 1930 and 1975, are followed by a rapid decrease until the late 1980s and then an increase from −25.0 to −23.0‰ through to the present day (Figure 2b).

Along the altitude transect, *Sphagnum magellanicum* $\delta^{13}C$ values range from −28.0 to −22.9‰ with a mean equal to −25.1 ± 1.57‰ (n = 12) for α-cellulose and from −28.4 to −23.5‰ with a mean equal to −26.0 ± 1.6‰ (n = 11) for bulk material (Figure 3). The $\delta^{13}C$ values of both fractions of modern specimens are correlated with altitude (Figure 3). For bulk plant material, the slope with respect to altitude is 1.8‰/km (significantly different from zero at the 1% level, $R^2 = 0.28$, n = 11). For α-cellulose, this slope is 1.7‰/km (significantly different from zero at the 1% level, $R^2 = 0.25$, n = 12).

Correlation coefficients among climatic variables themselves, temperature, relative humidity and atmospheric CO_2 concentration, are given in Table 2. Over the past 70 years, no correlation is found between humidity and atmospheric CO_2 concentration and between humidity and temperature (Table 2b). By contrast, temperature and $[CO_2]_a$ are strongly positively correlated. Along the altitude transect, humidity is significantly correlated with $[CO_2]_a$ and temperature. $[CO_2]_a$ and temperature are positively correlated, but less strongly than for the modern climatic conditions (Table 2a).

Data-model comparison

First, the measured and reconstructed Δ values are compared to test how well each of the equations estimates the overall effect of climate on discrimination. This test is done for the temporal (Figure 4, Table 3) and the spatial (Table 4) data sets. For the temporal data set, the coefficients of correlation between the measured and reconstructed Δ values are equal to 0.48 and 0.63 with the standard (equation (3)) and the mechanistic (equation (5)) approaches, respectively. These values increase up to 0.79 and 0.81 for the spatial data set. In both cases, a good reconstruction of Δ values general trends and range of variations is achieved (Figure 2).

The next step is to attempt to reconstruct individual climatic variables using the inverse forms of each of the three models. First, we use the standard and mechanistic approaches (equations (4) and (6), respectively). The results of these reconstructions are compared with instrumental values over the last 70 years (Figure 5). While the overall trends are adequately modelled, the variability of the reconstructed values is much larger than the variability of measured values for each climatic variable (temperature, humidity and $[CO_2]_a$). Furthermore, while reconstructed temperature and humidity show a consistent range of variations, the $[CO_2]_a$ calculations often yield unrealistic values.

Secondly, the reconstructed values for the climatic variables using the inverse mechanistic approach (equation (7)) are compared with instrumental values (Figure 5 and Table 3).

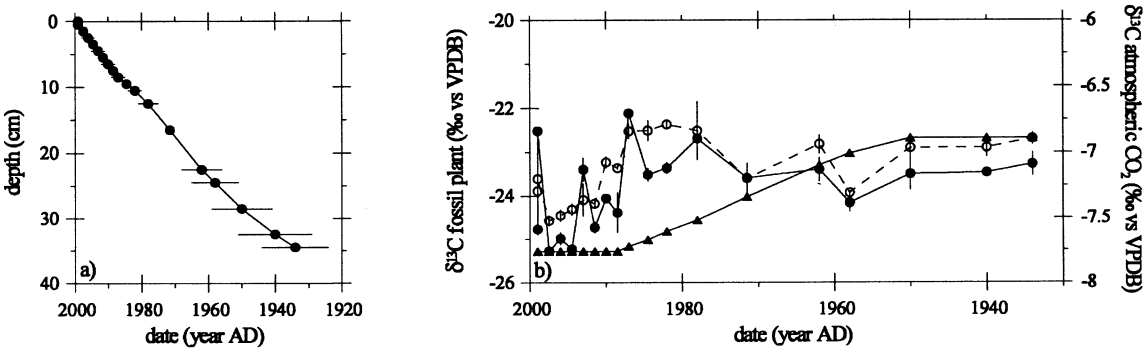

Figure 2 (a) Age-depth model for the peat core collected in Rötmoos (Figure 1). Closed circles represent individual ^{210}Pb datings. (b)Variations of *Sphagnum magellanicum* (circles) and atmospheric CO_2 (triangles) $\delta^{13}C$ values with time along this peat profile (palaeoclimate data set). Closed circles represent bulk material values. Empty circles represent α-cellulose values. Data show means obtained from at least three replicates, with their standard errors.

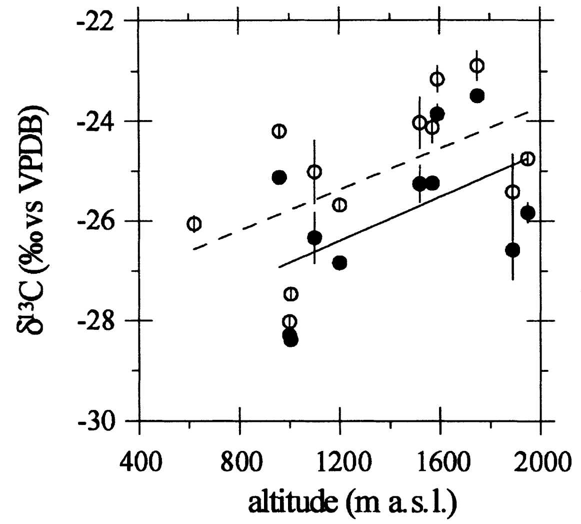

Figure 3 Variations of *Sphagnum magellanicum* $\delta^{13}C$ values with altitude along the spatial transect (Bernese Alps, Figure 1) (modern data set). Closed circles represent bulk material values and empty circles represent α-cellulose values. Data show means obtained from at least three replicates, with their standard errors. Solid and dashed lines represent the least square fits for bulk material (n = 11, $R^2 = 0.28$) and α-cellulose (n = 12, $R^2 = 0.25$) $\Delta^{13}C$ values, respectively.

Short-term variations of the predicted climate parameters are strongly reduced and much better fit instrumental values. The correlation coefficients between the instrumental and reconstructed values are much higher than those obtained with the traditional and mechanistic approaches ($R^2 = 0.83$, 0.99 and 0.77 for temperature, atmospheric CO_2 concentration and humidity, respectively; Table 3).

A similar approach can be applied to the spatial calibration data set: Δ values are compared to temperature, CO_2 concentration and relative humidity values along the altitude transect (Table 4). The standard method applied to spatial variations of Δ gives better results than when applied to temporal variations (Tables 3 and 4). However, the use of the mechanistic model again improves the quality of the reconstruction (Table 4). Finally, the inverse mechanistic approach leads to the best reconstruction of the three climatic variables, since the coefficient of correlation is then equal to 0.97, 0.98 and 0.66 for temperature, $[CO_2]$ and humidity, respectively (The values of the parameters estimated for the three models and the corresponding statistical significance tests are available upon request).

Table 2 Correlations between relative humidity (h), atmospheric CO_2 concentration ($[CO_2]_a$) and temperature (T), together with their statistical significance, for the temporal and spatial data sets, respectively

(a) Temporal calibration

n = 19	h	$[CO_2]_a$	T
h	1		
$[CO_2]_a$	−0.09	1	
T	−0.07	0.98*	1

(b) Spatial calibration

n = 23	h	$[CO_2]_a$	T
h	1		
$[CO_2]_a$	−0.98*	1	
T	−0.67*	0.63*	1

*Statistically significant at the 1% level, nonsignificant otherwise.

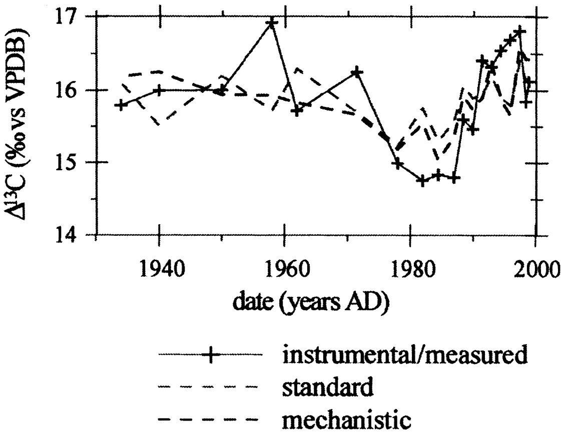

Figure 4 Observations (solid lines) compared to reconstructed values (dashed lines) of moss ^{13}C discrimination. The light grey and dark grey lines correspond to values reconstructed using the standard and mechanistic approaches, respectively.

Climatic control on moss discrimination

An estimate of the individual influence of temperature, relative humidity and CO_2 concentration on Δ when the other two parameters are held constant can also be derived from the mechanistic model using equation (8):

$$\begin{cases} \left(\frac{\partial\Delta}{\partial T}\right)_{h \text{ and } [CO_2]_a \text{cst}} = n_2 \log(h) + \frac{n_4 \log(h)}{[CO_2]_a} \\ \left(\frac{\partial\Delta}{\partial[CO_2]_a}\right)_{T \text{ and } h \text{ cst}} = -n_3 \frac{\log(h)}{[CO_2]_a^2} - n_4 \frac{T \log(h)}{[CO_2]_a^2} \\ \left(\frac{\partial\Delta}{\partial h}\right)_{T \text{ and } [CO_2]_a \text{ cst}} = \frac{n_1}{h} + n_2 \frac{T}{h} + \frac{n_3}{[CO_2]_a h} + \frac{n_4 T}{[CO_2]_a h} \end{cases} \tag{8}$$

We can estimate the variations of Δ induced by changes of temperature and $[CO_2]_a$ for a given humidity (Figure 6). In the range of climate parameters encountered over the temporal calibration set, temperature has a negative effect on Δ (when temperature increases, Δ decreases) for small values of $[CO_2]_a$, while the opposite is true for high values of $[CO_2]_a$ (Figure 6a). Similarly, at low temperature values, Δ decreases as $[CO_2]_a$ increases and the opposite is true at high temperature (Figure 6a). When the influence of temperature and $[CO_2]_a$ on Δ is considered along the altitude transect (Figure 6b), the slope has a constant sign, positive for both variables. Furthermore, the impact of temperature on Δ is greater at low than at high $[CO_2]_a$ values (Figure 6b). Similarly, the impact of $[CO_2]_a$ is more positive at low than at high temperature values (Figure 6b). Similar reconstruction is done for the impact of humidity

Table 3 Correlation coefficients between measured/instrumental and reconstructed values of Δ, temperature, atmospheric CO_2 concentration and relative humidity. Three approaches are compared: the traditional, the mechanistic and the inverse mechanistic approaches. Two numbers of the correlation coefficient between instrumental and reconstructed $[CO_2]_a$ are given: the first one corresponds to the complete data series, whereas the number in brackets is obtained without four extreme data points

Temporal calibration

n = 19	Δ	T	$[CO_2]_a$	h
	Measured/ reconstructed		Instrumental/ reconstructed	
Traditional	0.48	0.50	0.36	0.19
Mechanistic	0.63	0.44	0.024 (0.39)	0.18
Inverse mechanistic		0.83	0.99	0.77

Table 4 Correlation coefficients of measured/instrumental and reconstructed values of $\Delta^{13}C$, temperature, atmospheric CO_2 concentration and relative humidity. Three approaches are followed: the standard, mechanistic and inverse mechanistic approaches (details in text)

Spatial calibration

n = 19	Δ	T	$[CO_2]_a$	h
	Measured/ reconstructed	Instrumental/ reconstructed		
Traditional	0.79	0.70	0.91	0.58
Mechanistic	0.81	0.92	0.97	0.75
Inverse mechanistic		0.97	0.98	0.66

variations when either $[CO_2]_a$ or temperature is fixed (results not shown). Humidity is found to have a positive effect on Δ for the entire range of temperature and $[CO_2]_a$ for both data sets. These results indicate that assuming a constant relationship between a climate parameter and isotopic response is not likely to be valid. Yet this assumption is the basis of most isotopic palaeoclimate reconstructions.

Another way to reconstruct the quantitative relationship between Δ and meteorological parameters using the mechanistic approach consists in using equation (8) and the values of the parameters estimated. The effect of each climate parameter is calculated for the two data sets in two ways: (1) at given altitude and date (540 m in 1999) over the altitude transect; (2) at average conditions over time. The values obtained are compared to their effect expected from the literature (Table 5). A positive impact of temperature when estimated over time and a negative one when estimated along the altitude transect is found. The inverse is true for humidity, but the effect is small when estimated over time. Last, the effect of CO_2 on Δ is positive except at mean conditions when estimated across time (small and negative). Thus climate-isotope calibrations based on spatial variations may not be valid for reconstructing temporal variation in climate. Again, this method is commonly used in palaeoclimatology.

Discussion

Mechanistic versus traditional approaches

First, quantitative relationships between isotopic ratios and environmental parameters are most often derived from linear regressions (Edwards *et al.*, 1985; Lipp *et al.*, 1996) in which each climate parameter is treated independently from others. Using a mechanistic model, in which climatic variables are not independent, to derive the estimated equation significantly improves the correlation between measured and modelled estimates of carbon isotope discrimination (Tables 3 and 4). Standard linear regressions may also be biased by the correlations commonly observed between climatic variables. As an example, in our study CO_2 concentration is strongly negatively correlated with humidity along the altitude transect, and positively with temperature during the last 70 years (Table 2). This makes difficult the estimation and interpretation of the impact of climate parameters introduced independently in regressions as assumed by the standard approach. The mechanistic model shows that each climatic variable works in combination with the two others. For example, in the mechanistic model the influence of temperature on Δ depends on the humidity and CO_2 concentration conditions experienced by plants (see equation (8)), whereas it is constant (equal to m_2; see equation (3)) in the standard linear regression approach.

Secondly, the inverse mechanistic approach improves the reconstruction of climatic variables. Statistical methods used to estimate empirical relationships minimize the error on the dependent variable (Δ for both the standard and mechanistic approaches). Thus, observed and modelled values of Δ are in good agreement (Figure 5a). However, when the equation is inversed to reconstruct a climatic variable, the error on this variable is not necessarily minimized and some extreme values are observed (Figure 5). In particular, short-term variations of climatic variables are poorly predicted, even though average trends are well described. This difficulty is circumvented by the inverse mechanistic approach that estimates a relationship in which the climate parameter to be predicted is the dependent variable (see, for example, equation (5)). Our results show that a significantly better reconstruction is achieved with this approach (Figure 5, b and c).

Palaeoclimate reconstruction: temporal versus spatial calibration

The calibration of the transfer function between carbon discrimination and humidity, temperature and CO_2 concentration on both the temporal and the spatial gradients allows us to provide some comparisons between these two ways of assessing the impact of climatic variables on isotope records. Spatial relationships between climatic and isotopic variation, because they are easily determined, are often applied to reconstruct

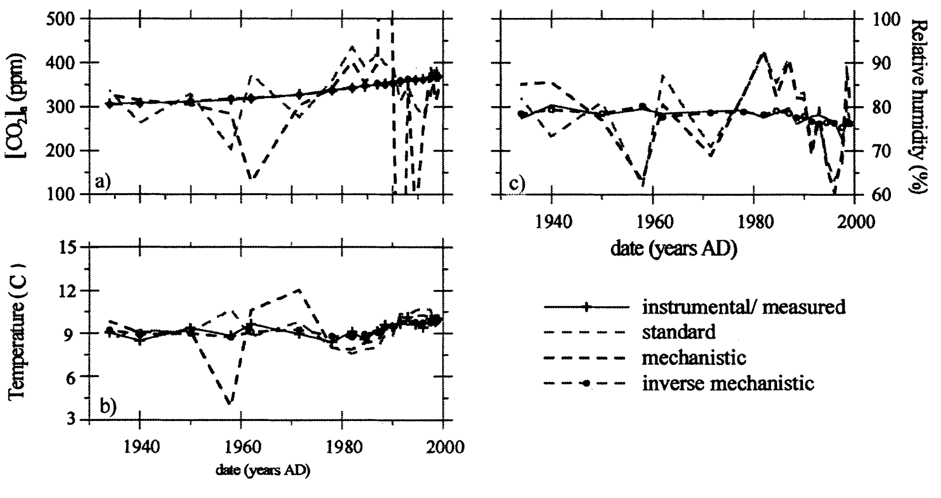

Figure 5 (a) Temperature, (b) CO_2 concentration and (c) humidity. The light grey, dark grey and thick (with dots) lines correspond to values reconstructed using the standard, mechanistic and inverse mechanistic approaches, respectively.

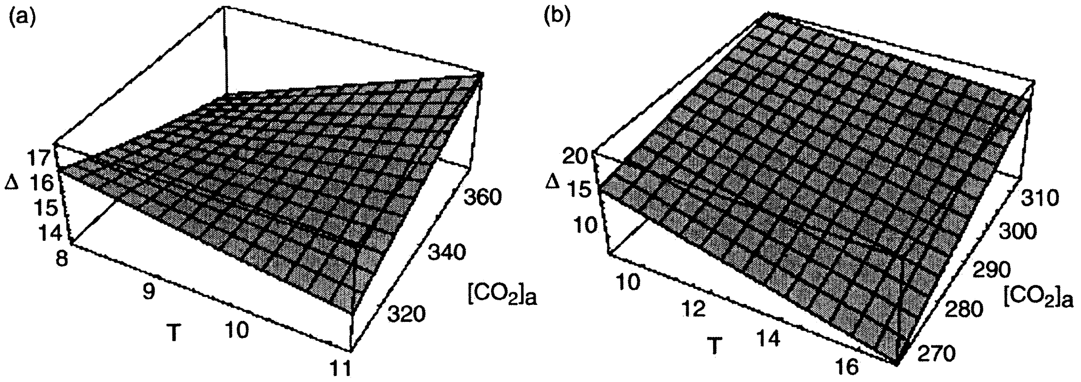

Figure 6 Δ against temperature and $[CO_2]_a$ for given humidity: effect of temperature and $[CO_2]$ at constant value of humidity inferred from (a) the palaeoclimate data set and (b) the modern data set. These estimations are calculated using the values of the parameters n_1, n_2, n_3 and n_4 estimated on both data sets and equation (5). For instance, each line from the surface parallel to the T-axis represents the variation of Δ due to T and $[CO_2]_a$ at h constant.

temporal climatic variation. However, our results show that the effect of climate parameters on discrimination may differ not only in magnitude but also in sign between temporal and spatial data sets (previous section; Table 5).

As an example, we obtain contradictory temperature/discrimination relationships with the temporal and spatial calibrations (Table 5) or, more generally, depending on the values of other climatic variables (Figure 6). To our knowledge, no laboratory study has examined the relationship between temperature and $\delta^{13}C$ discrimination of mosses. However, because mosses and vascular plants use the same photosynthetic pathway, temperature might be expected to influence them in the same way. A number of field and laboratory studies have attempted to quantify the effect of temperature on plant metabolism. Surprisingly, the results of experiments done under controlled conditions almost universally disagree with field results. In contrast, results from our temporal calibration data set are in agreement with the laboratory (Morecroft and Woodward, 1990; O'Leary, 1988) and a few field studies (Leavitt and Long, 1982; Edwards *et al.*, 2000) showing a negative correlation between temperature and $\delta^{13}C$. Similarly to most field studies (see, for a review, Ménot and Burns, 2001; Schleser *et al.*, 1999), the opposite is suggested by the spatial calibration.

One explanation for these apparently puzzling results may be that the influence of temperature (or any of the climatic parameters) is nonlinear. The problems linked to the nonlinearity of the Δ response to parameter changes were reviewed by Schleser *et al.* (1999). The influence of temperature depends on the values of humidity and CO_2, as underlined by the mechanistic model. Furthermore, the ranges of climate parameter variations greatly differ in the spatial, where climatic variation is large, versus the temporal, where it is small, data sets. Temperature changes by about 8°C along the altitude transect, whereas it shows a variation of only 1–2° over the past 70 years. By contrast, humidity varies slightly along the altitude transect as well as over time. The impact of temperature for given values of $[CO_2]_a$ and humidity is then different when estimated on the temporal or spatial calibration sets (Table 5).

Table 5 Effects of humidity, temperature and atmospheric CO_2 concentration on moss $\Delta^{13}C$. The estimated effects are compared with those expected from the literature (see reference in text). For each data set, the estimations are computed using equation (4), the estimated values of n_1, n_2, n_3 and n_4, and the average values of the climate parameters (over the last 70 years and along the altitude transect)

	Expected effect on Δ	Estimated effect on Δ	
		Temporal calibration (in 1999/ temporal mean)	Spatial calibration (in Bern /spatial mean)
T	?	1.3/0.61	−0.32/−0.72
$[CO_2]_a$	+	0.01/−0.01	0.17/0.15
h	−	−0.05/−0.05	0.39/0.38

This discrepancy in the translation of variations in climate parameters in $\delta^{13}C$ between the two data sets might also be interpreted as different physiological response of mosses to environmental changes associated with two different situations. Along the altitude transect, plants are genetically adapted to the spatial variations of climate parameters encountered (Körner *et al.*, 1991). On the other hand, along a peat profile, temporal changes for which plants may not be adapted may be encountered.

Future research

We would first like to underline that the approach we develop is applicable not only for carbon isotopes in plants but also for oxygen or deuterium isotopes. More generally, any proxy that is related to climate changes through a theoretical model could be estimated in this way, which would improve the quality of the estimations and of the reconstructions of climates.

We have underlined that temporal and spatial data sets do not yield the same impact of climatic variables on Δ. This was a first sign that using spatial calibrations to make temporal reconstruction might lead to poor results. Our further investigations confirm that it is problematic to reconstruct past climatic variations strictly using relationships derived from spatial calibrations, even using the mechanistic or the inverse mechanistic approaches. We have tested this approach in two ways: by reconstructing past climatic variation from spatial calibration, and by reconstructing spatial variation from the temporal calibration. Although the data are not shown, we found almost no correlation between the measured and the reconstructed values of climate parameters in both cases. Wherever possible, it appears therefore much more appropriate for the prediction of future climatic variations to calibrate the transfer functions using a temporal data set. At least, if one wants to use estimation along an altitude transect to forecast past or future variations in a given place, the spatial data set used has to reflect as closely as possible the range of climatic variations to be predicted. Our results show that not only should the temperature have the same amplitude of change but also the other climatic parameters (humidity and $[CO_2]_a$), in order to get a correct estimation of the equation. This would take care only of the potential statistical bias; the problem of the physiological adaptation first mentioned by Körner *et al.* (1991) remains.

One drawback of the inverse mechanistic approach is that a given climate parameter is reconstructed using not only observed Δ values but also the two other climate parameters. Such information is not always available. A promising line of future research would consist of using two other mechanistic models for $\delta^{18}O$ and δD. Then one would solve the three-equation system to express each climate parameter as a function of Δ, $\delta^{18}O$ and δD only. Once estimated, such an equation would enable the reconstruction of any climate parameter without using the other ones.

Conclusions

We conducted a study of ^{13}C discrimination on a moss species, *Sphagnum magellanicum*, commonly found in temperate and tropical peat bogs. Both modern and fossil plant samples were analysed to provide both a temporal and a spatial calibration set of data. Our results confirm that, as humidity increases and atmospheric CO_2 concentration decreases, $\delta^{13}C$ increases. Furthermore, the relationships between moss $\delta^{13}C$ on the one hand and humidity, CO_2 concentration and temperature on the other reveal that the temperature is found to have a negative influence on $\delta^{13}C$ (as temperature decreases, $\delta^{13}C$ increases). We, however, find that the magnitude and, in some cases, the sign of the impact of one climatic variable depends on the calibration set considered.

Multiple regression is a useful tool to assess the relationships between different variables. However, the interpretation of the estimated statistics can be complicated by correlation between variables considered as the explanatory variables in the multiple regressions. The use of a mechanistic model greatly helps in specifying the joint influence of the climatic variables.

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Note

Parameters n_1, n_2, n_3 and n_4 are functions of the constants of the model of Figge and White (1995) where W(h) is taken to be the natural logarithm of humidity and W_{dry} is set to zero, as suggested by Proctor (1982):

$$n_1 = -(b-a)\frac{rP^0_{max}}{W_{opt}}(1-\lambda T_0)\beta, n_2 = -(b-a)\frac{rP^0_{max}}{W_{opt}}\lambda\beta,$$

$$n_3 = -(b-a)\frac{rP^0_{max}\alpha}{W_{opt}}(1-\lambda T_0), n_4 = -(b-a)\frac{rP^0_{max}}{W_{opt}}\lambda\alpha$$

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