Improving Alkenone Temperature Paleoclimate Reconstruction, with Example from the Last Glacial Maximum Tropics

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Abstract

Using an up-to-date carefully-compiled ocean sediment core alkenone time series database it is shown that there is a widespread assumption that an inversion of a spatial (e.g., global) calibration equation (e.g., Müller et al., GCA **62** (1998), 1757) relating the alkenone index (e.g., $U_{37}^{K'}$) to present day SST somehow correctly accounts for all factors through the past such that it can be used as a temporal (paleo) SST equation at individual core sites. The assumption is shown to only seem valid superficially and to be wrong conceptually, mathematically, through close analogy with ice cores, and using a better paleoclimate reconstruction method. The method, using $U_{37}^{K'}$ as a temperature proxy, is to do the best possible paleosimulations with the most sophisticated global climate models to physically-consistently take care of the climate factors, input the results to a proxy model of how $U_{37}^{K'}$ is affected by climate and other factors and then directly validate the results with a large global $U_{37}^{K'}$ paleorecord database. With this method, the $U_{37}^{K'}$ versus water temperature only relationship of culture calibrations is fundamental and critical. The most-used one is a linear regression/extrapolation from Prahl et al. (GCA **52** (1988), 2303). It is shown, particularly in the tropics where it is often used outside its valid range, that never-used non-linear regressions/extrapolations of it may be better, calling into question many previous alkenone SST paleoclimate reconstructions. An example using the better method is done for the LGM tropics and LGM minus present day SST are estimated there. Alkenones then seem to be consistent with climate models in this CLIMAP-instigated controversy and indicate a significant SST difference.

1. Introduction

Reconstruction of paleoclimate, including paleoceans, is typically done using either primarily climate modelling or primarily climate proxies. Paleoclimate proxy researchers get proxy data, from ocean sediment cores for example, from just a few sites and from this data, which is the result of an unknown combination of numerous factors, infer large-scale climates. Conversely, paleoclimate modellers simulate large-scale climates, often using the same climate models as for future climate prediction and the results of which are just physically-consistent, not necessarily true, and validate with just a few proxy-based inferences, if at all. Even though they are necessarily-connected, proxies and modelling tend to be separate fields that may not fully appreciate the assumptions made by the other, which can lead to problems, as shown in this work. Neither can be said to be better and in fact they are at their best when in reconstructing paleoclimate they are as integrated as possible, as also shown in this work. In this work, the ocean temperature proxy of alkenones from ocean sediment cores is used. This is a good proxy to start to do the preceding with because it is relatively simple compared to other proxies (for description see review of Herbert (2003) and references therein).

2. Alkenones

Alkenones are organic compounds produced in the present day ocean by haptophyte (phylum Haptophyta or Prymnesiophyta) phytoplankton (single-celled algae). They are primarily produced by the ubiquitous and abundant marine coccolithophorid (covered in calcite platelets, known as coccoliths) species *Emiliania huxleyi* (class Prymesiophyceae, order Isochrysidales, family Noelaerhabdacae) but the rarer coccolithophorid species *Gephyrocapsa oceanica* (same family) may be important regionally.

The Ketone Unsaturation index, $U_{37}^{K'}$ (specifically, Prahl and Wakeham, 1987), is the ratio of the concentration of di-unsaturated long-chain C_{37} ketones, [37:2], to the concentration of the total of di-unsaturated C_{37} ketones and tri-unsaturated C_{37} ketones, [37:3]:

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$$U_{37}^{K'} = \frac{[37{:}2]}{[37{:}2 + 37{:}3]} \quad (1)$$

Long-chain C_{37} ketones are alkenones with 37 carbon atoms and the n-saturation refers to the number of double bonds. $U_{37}^{K'}$ is a simplified version of an earlier index, U_{37}^{K} (Brassell et al., 1986), that includes tetra-unsaturated C_{37} ketones, $C_{37:4}$:

$$U_{37}^{K} = \frac{[C_{37:2}] - [C_{37:4}]}{[C_{37:2} + C_{37:3} + C_{37:4}]}$$

Tetra-unsaturated C_{37} ketones occur only in cold waters, such as the high-latitude North Atlantic, but rarely in the Southern Ocean. U_{37}^{K} is used but there are few alkenone records from those regions. Elsewhere, there is so little $C_{37:4}$ that U_{37}^{K} is mathematically equivalent to $U_{37}^{K'}$ and/or they are simply ignored and $U_{37}^{K'}$ used. Because of this U_{37}^{K} will not have to be considered in this work.

Early work with cultures of *E. huxleyi* grown in the laboratory showed that $U_{37}^{K'}$ is monotonically positively related to the water temperature (T) the phytoplankton were growing in when they produced the alkenones. Prahl et al. (1988) was early culture work and is still by far the most-used culture calibration of $U_{37}^{K'}$ versus production temperature. Via least squares analysis of their five data points — $U_{37}^{K'}$ from culture experiments at five different water temperatures 8 to 25°C — they got the linear relationship

$$U_{37}^{K'} = 0.034 * T + 0.039 \quad (2)$$

Inverting Eq. 2 would then for an observed $U_{37}^{K'}$ value give the temperature of the water the phytoplankton were growing in when they produced the alkenones:

$$T = \frac{1}{0.034}(U_{37}^{K'} - 0.039) = 29.4 * U_{37}^{K'} - 1.15 \quad (3)$$

3. Complicating Factors

Alkenone-producing phytoplankton inherently tend to live in the photic zone, so usually at some depth from the thermocline to the sea surface, but mostly nearer the latter where the sunlight is least attenuated. The temperature of the water the phytoplankton are growing in when they produce the alkenones would thus tend to be close to sea surface temperature (SST). Early and later work generally found a good correlation between $U_{37}^{K'}$ and present day mean annual SST so this has become assumed. The phytoplankton die and some portion of the alkenones eventually sink and accumulate over time in the ocean sediments, presumably leaving a paleorecord of the mean annual SST over the ocean sediment site.

However, there are factors that can mean $U_{37}^{K'}$ does not give mean annual SST over the site it is observed at and so greatly complicate using $U_{37}^{K'}$ records to reconstruct paleoclimate, which is the goal. Most of the most important of these complicating factors are climate related, most directly to the ocean part of climate. All factors, and their combination, can vary regionally and change on the time scales that climate changes. The factors may only be important regionally and not globally but since the concern is individual ocean sediment core sites they must be considered, especially since core sites tend to be in locations with a lot of variability, like along coasts, rather than in the more stable mid-ocean. For a more complete outline of these complicating factors see the review of Herbert (2003) and references therein. Only the most important ones will be mentioned here, with no discussion of factors for which it is even questionable whether they would affect the alkenone ratio (preservation in sediments for example). For the purposes of this work, it should be noted that all of the factors have the possibility of being modelled.

First, the exact depth the phytoplankton were living at when they produced the alkenones is actually unknown. While as indicated it is assumed to usually be in the uniform-temperature surface mixed layer, so that the water is at SST, it can be deeper, into the thermocline, and thus colder by several degrees. Further, the phytoplankton may live at different depths during their lives, depending for example on ocean circulation changes, and the temperature contribution from each habitat depth has to be considered when interpreting $U_{37}^{K'}$.

Second, the exact time of year the preserved alkenones were produced is actually unknown. Phytoplankton tend to grow in blooms and these would be expected to have the greatest effect on sediment $U_{37}^{K'}$, which will be some time average. Typically such blooms have been observed to occur during the spring months, when SST are about the same as mean annual SST, which results in the noted correlation. However, these blooms can be shifted into the summer months, due for example to ocean circulation changes like upwelling. The blooms can also last more than a month, during which SST can change significantly, and the temperature contribution from each month has to be considered when interpreting $U_{37}^{K'}$. Note that orbit-related millennial-scale climate changes are often a matter of seasonal changes.

Third, not only is it not known vertically exactly where the phytoplankton were living when they produced the alkenones but it is not known laterally. Before alkenones come permanently to rest in the ocean sediment they can be significantly transported away from their production site and change in an unknown way the $U_{37}^{K'}$, and thus temperature, seen at the site where they finally come to rest. Benthien and Müller (2000) is an oft-cited example from the Malvinas Current region of the western South Atlantic. Whether from transport before or after first reaching the ocean sediment this transport is obviously strongly dependent on ocean circulation, which can change over time.

Finally, while *E. huxleyi* is the most significant alkenone producer worldwide today, there are some regions where *G. oceanica* is and where both are significant contributors. Further, this distribution was different in the past, with for example, *G. oceanica* globally dominant during some periods before the evolutionary appearance of *E. huxleyi* approximately 265 ka. All this is important because *G. oceanica* may have a different $U_{37}^{K'}$ versus production temperature relationship than *E. huxleyi* (e.g., Volkman et al., 1995).

4. Assumption of Spatial Calibration Equations

A spatial calibration of two variables, here $U_{37}^{K'}$ and SST, is done using observations of them over a region or globally in order to include the relevant variation, usually caused by numerous factors, here including the major ones described in Sec. 3. The observations are "present day" since otherwise all that is available are proxies, which the calibration is usually done for in the first place. Unfortunately, there is an assumption that an inversion of a spatial calibration equation relating $U_{37}^{K'}$ to present day SST somehow correctly accounts for all factors through the past such that it can be used as a temporal (paleo) SST equation at individual ocean sediment core alkenone paleorecord sites.

Müller et al. (1998) is a more-recent calibration that is next most used (by far) in alkenone temperature paleoclimate reconstructions, the point here, compared to Prahl et al. (1988). However, unlike Prahl et al. (1988) Müller et al. (1998) is not a culture calibration. It is a global (i.e., spatial) sediment coretop calibration to present day mean annual SST:

$$U_{37}^{K'} = 0.033 * \mathrm{SST} + 0.044 \quad (4)$$

As such it is assumed to account for all the complicating factors through the past when inverted to calculate a past mean annual SST from a $U_{37}^{K'}$ value in an ocean sediment core paleorecord:

$$\mathrm{SST} = \frac{1}{0.033}(U_{37}^{K'} - 0.044) = 30.3 * U_{37}^{K'} - 1.33 \quad (5)$$

An up-to-date database of ocean sediment core alkenone time series has been carefully compiled (see Appendix 1 for further description). This includes only those paleorecords that have publications that document how they were produced. The main point of almost all of the alkenone papers is to try to reconstruct paleoclimate with SST calculated from alkenone ratios. The inverted calibration equation used for each core, and why, has been carefully noted. Among the 58 papers (77 cores), 35 papers (46 cores) used the inverted calibration equation of Prahl et al. (1988) but of these, 12 papers (18 cores) noted or implied that it was essentially the same as that of Müller et al. (1998) and 12 papers (15 cores) were published in or before 1998, and even 4 papers (5 cores) of these made the comparison to earlier spatial calibrations. Conversely, 15 papers (21 cores) used the inverted calibration equation of Müller et al. (1998) but of these, 3 papers (6 cores), including Müller et al. (1998) itself, noted or implied that it was essentially the same as that of Prahl et al. (1988) and 1 paper (2 cores) even made the comparison to an earlier culture calibration.

Much has been made of the apparent equivalence within error limits of the Müller et al. (1998) (or other) spatial calibration and the Prahl et al. (1988) (or other) culture calibration, particularly as if this validated the former. A good summary of the whole situation is given in the recent alkenone paleothermometry review of Herbert (2003) (first paragraph of Sec. 6.15.7 on Pg. 412):

> The resemblance of core-top alkenone unsaturation data to both mean annual SST and the original Prahl *et al.* (1988) culture calibration is a quite remarkable result that is not completely understood. As the review above suggests, the calibration of a temperature proxy for paleoenvironmental analysis involves a host of steps, ranging from the physiology and genotype of the producing organisms, their ecology, and eventually the transport and degradation of particles in the water column and sediments. In the case of the alkenone thermometer, it is comforting to note that water-column and sediment calibrations come quite close. The consistency of the sediment regression to the original Prahl *et al.* (1988) linear relation is in some sense fortuitous. Other culture studies produce results that differ as much as 5°C from the standard Prahl *et al.* (1988) calibration, and there is no inherent reason to prefer a linear calibration of unsaturation to growth temperature to a nonlinear one. Further, we know that alkenone producers do not operate at constant rates throughout the year in most regions of the ocean, and that they do not always live in the mixed layer. One should therefore keep in mind that the Prahl *et al.* (1988) and the identical Muller *et al.* (1998) relation of $U_{37}^{k'}$ with the mean annual SST are idealizations.

This situation seems to have provided support for concentrating on using spatial calibrations instead of culture calibrations. For example, of the remaining 8 papers (10 cores) in the database, all after 1998, 7 papers (9 cores) used regional (spatial) coretop sediment calibrations; only 1 paper (1 core) used a culture calibration and that calibration even predates Prahl et al. (1988). Further, there has continued to be a significant amount of work on developing spatial calibrations (e.g., Conte et al. (2006) and references therein), perhaps to the detriment of work on or with culture calibrations.

5. Why Assumption Is Wrong

Conceptually, there is simply no clear physical reason why the present day spatial change in the complicating factors (Sec. 3), or especially their combination, should be the same as the temporal (paleo) change in the factors, or their combination especially, at an individual site. For example, this might just coincidentally equate, via temperature alone, a more-poleward present day site with the site at the LGM and these two sites might always have very different combinations of complicating factors.

Stated mathematically, what is usually sought is a single or just a few equations to calculate SST from $U_{37}^{K'}$ at any ocean sediment core site at any past time:

$$\mathrm{SST} = \mathrm{a} * \mathrm{U}_{37}^{K'} + \mathrm{b} \tag{6}$$

However, the mere occurrence of T and $\mathrm{U}_{37}^{K'}$ in an equation does not mean it can be used for this, i.e., just inverting any calibration equation relating $\mathrm{U}_{37}^{K'}$ to T (a linear equation is used here only for reasons of simplicity and familiarity, since linear regression is the most popular choice in such calibrations; the specific form of the equation is irrelevant to the argument). Assuming a single or just a few equations could be valid globally or over regions (i.e., spatial calibration), respectively, at any time, the coefficients, which parameterize the complicating factors, would almost certainly be functions of time in the past (t). Again, a priori, there is simply no clear physical reason to assume otherwise. Actually then, Eq. 6 is

$$\mathrm{SST} = \mathrm{a}(t) * \mathrm{U}_{37}^{K'} + \mathrm{b}(t) \tag{7}$$

And equations from present day (t_0) spatial calibrations are

$$\mathrm{SST} = \mathrm{a}(t_0) * \mathrm{U}_{37}^{K'} + \mathrm{b}(t_0) \tag{8}$$

where t_0 is actually a temporal average, perhaps a few thousand years at worst using ocean sediment coretops. Equating Eqs. 6–8 is the same as saying there is no change in climate in the past, i.e., modelling past climates simply as the present day climate. If this were true, no past changes in SST and $\mathrm{U}_{37}^{K'}$ should be expected. Note that it might be said that currently most paleoclimate reconstruction from proxies already involves climate models — but simplistic conceptual models or just inverted calibration equations. The use of spatial calibrations has a present day model built in.

As a very close analogy, ice cores also indicate this assumption is wrong and, being more validated, provide a compelling cautionary tale.

The isotopic ratio, δ^{18}O, in ice core H_2O of rare heavy oxygen, ^{18}O, to common light oxygen, ^{16}O, has been a very important proxy in determining past surface air temperatures, T_S. The connection though, between surface air temperature and precipitation δ^{18}O, and thus ice core δ^{18}O, is complicated and very similar to SST and $\mathrm{U}_{37}^{K'}$ in ocean sediment cores. Also similarly, to relate past T_S and ice core δ^{18}O a linear present day spatial calibration equation is typically used. An early but still oft-used one is from Dansgaard (1964) who linearly calibrated precipitation δ^{18}O from various temperate to polar sites against present day mean annual surface air temperatures there:

$$\delta^{18}\mathrm{O} = 0.69 * \mathrm{T}_S - 13.6 \tag{9}$$

Presumably it was used because there was simply no other possibility yet in paleotemperature calculation, such as will be described in this work. Inverting Eq. 9, the past mean annual surface air temperature indicated by a δ^{18}O value in an ice core record is then calculated as

$$\mathrm{T}_S = \frac{1}{0.69}(\delta^{18}\mathrm{O} + 13.6) = 1.45 * \delta^{18}\mathrm{O} + 19.7 \tag{10}$$

All of the preceding arguments for ocean sediment cores alkenones also apply to this analogous ice core situation. However, further validations on ice cores have been done and these very convincingly — via the magnitude of the erroneous conclusions drawn — imply that the use of an inverted spatial calibration equation is wrong. Only the important relevant points will be recounted here; for a more-detailed description see Thresher (2004) (Sec. 7.4) and references therein or the earlier Broecker (2002).

Borehole paleothermometry has been applied to the GRIP and nearby GISP2 ice core boreholes in Greenland. When the Last Glacial Maximum (LGM; 21 ± 1.5 kyr BP) ice core δ^{18}O values are put in an equation like Eq. 10 (i.e., a linear equation with constants slightly modified specifically for Greenland), an LGM mean annual surface air temperature of about -41°C is concluded. However, borehole paleothermometry gives about -50°C. Since the present day mean annual surface air temperature at the site is about -32°C, this 9°C discrepancy is very significant.

General circulation models (GCM; the most sophisticated global climate models) that fully carry (i.e., account for all their complicated physics/dynamics) the oxygen isotopes in their hydrological cycles have also been applied. The results remarkably bear out those above from borehole paleothermometry (Werner et al. (2000), using an atmosphere-only GCM, and Thresher (2004), using a full coupled atmosphere-ocean GCM).

These results clearly show that for ice cores an inversion of a spatial calibration equation relating δ^{18}O to present day surface air temperature is not valid as a paleotemperature equation at individual ice core sites. Further, such equations have been used extensively (on most ice cores) and given the magnitude of the errors have thus been very confusing to paleoclimate reconstruction. There may be the same consequences from current similar practice for alkenones in ocean sediment cores.

6. Why Assumption Seems Valid

Superficially it might seem that the Müller et al. (1998) spatial calibration equation being essentially identical to the Prahl et al. (1988) culture calibration equation is remarkable, some sort of validation of spatial calibrations. Looking just a little deeper, as was initially done for this work, and finding that mean annual SST generally varies monotonically with equator-to-pole latitude, in mid-latitudes often linearly with a 1 °C/°latitude slope, one might be tempted to see that as directly part of the reason. However, the probable real reason is actually simpler, as follows.

Spatial calibrations are like doing numerous culture experiments at different water temperatures, although also including the regional complicating factors (Sec. 3). The Müller et al. (1998) data spans the latitude range 60°S to

60°N and thus the temperature range 0–29°C, completely encompassing and going beyond the 8–25°C range of the Prahl et al. (1988) culture calibration. With hundreds of globally distributed data points, the regional complicating factors tend to cancel out or be dwarfed, leaving just a $U_{37}^{K'}$ versus production (water) temperature (only) relationship of a culture calibration. It would actually be remarkable if Müller et al. (1998) was not essentially identical to a globally representative culture calibration. And the Prahl et al. (1988) culture calibration was done with the globally-predominant alkenone-producing species, *E. huxleyi*, over a large part of the Müller et al. (1998) temperature range. Although Prahl et al. (1988) itself and Sawada et al. (1996) provide some evidence, there is still the question of whether the strain of species used in Prahl et al. (1988) is globally representative. However, given the validity of the rest of the argument made here, it may be that the similarity of Müller et al. (1998) and Prahl et al. (1988) is evidence itself concerning these issues. Further then, the discrepancies between Müller et al. (1998) and Prahl et al. (1988) tend to come where Müller et al. (1998) is outside the temperature range of Prahl et al. (1988); why this is especially true will be discussed in Sec. 8.

A perhaps enlightening thought experiment, analogous to the current situation, is to consider several hundred random water temperature values between 0 and 29°C; being random they will contain no climate information. Convert these to $U_{37}^{K'}$ values using Prahl et al. (1988) (Eq. 2). Just before or after these conversions, make just a few "regional" values a little larger or smaller and/or some larger and some smaller. Next do (Müller et al., 1998) a linear regression of the resulting $U_{37}^{K'}$ values against the water temperature values. The result is going to look much like Prahl et al. (1988) (Eq. 2). The effects of the "regional" variations are lost.

Note that the loss of the effect of the regional complicating factors when using a global calibration equation is part of the reason such an equation is not valid at the site of an individual ocean sediment core, which is what is sought. Illuminatingly, according to Pelejero and Calvo (2003), the Benthien and Müller (2000) alkenone data with large temperature biases due to lateral transport was, for that reason, not included in the global compilation of coretop data. This is a purposeful loss of a regional complicating factor in a spatial calibration and is not known whether this factor existed there or anywhere else in the past.

Finally, note that suggested (e.g., Conte et al. (2006) and references therein) changes of spatial calibrations, regional instead of global for example, may make them less like globally representative culture calibrations and thus actually harmful to the better use of alkenone temperatures for paleoclimate reconstruction.

7. Better Paleoclimate Reconstruction Method

Given all the preceding, a better method is necessary to use the alkenone index as a temperature proxy and reconstruct paleoclimates. One idea is to additionally use other proxies from the same site (i.e., ocean sediment core) to separate out the complicating factors. However, this still leaves the fundamental proxy limitation of using data from just a few sites to infer large-scale climate. A better method then is to do the best possible paleosimulations with the most sophisticated global climate models to physically-consistently take care of the climate factors, input the results to a proxy model of how the alkenone index is affected by climate and other complicating factors and then directly validate the results with a large global database of alkenone index paleorecords. Fig. 1 is a schematic of the general method, which is also called or is a form of or is related to (depending on how it is defined), "forward modelling".

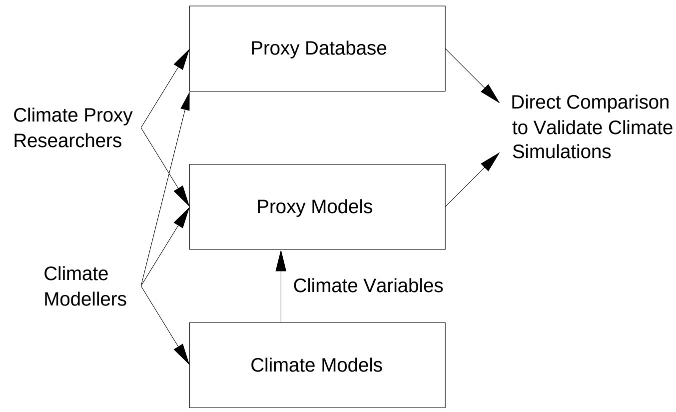

Fig. 1. Schematic of better paleoclimate reconstruction method.

Doing the "best possible" paleosimulations means, for example, using boundary conditions as appropriate as possible for the simulated time slice. The need for this and using the "most sophisticated" global climate models is because of the need to try to match the proxy paleorecords sufficiently accurately to be useful.

With this method, the alkenone index versus production temperature (only) relationship of culture calibrations is fundamental and critical and indeed this work was done while beginning to develop an alkenone index proxy model. The best culture calibrations should thus also be used, with "best" meaning most appropriate, including in the past, for the species and strains in a region and the estimated maximum possible temperature range there.

With this method, if the proxy model is separate (i.e., offline) from the climate model, then it can be used with various climate models to see whose paleosimulations best match the proxy database. As will be exemplified in this work, the method has other benefits as well, besides providing a common reference frame for comparisons, such as bringing together knowledge about the proxy (while developing its model), allowing relatively easy experimenting (with the model) to learn about the proxy, and predicting critical sites for getting the proxy data.

8. Use of Culture Calibrations

Again, for this better method the $U_{37}^{K'}$ versus production temperature (only) relationship of culture calibrations is fundamental and critical and the one most used by far for paleoclimate reconstruction, the point here, is Prahl et al. (1988). It may be that it is the most used because it is early work and because of the described superficial validation. For the same reasons it may not have been fully considered before. Other newer culture calibrations should be considered (e.g., Conte et al., 1998) and in fact this is being done as part of developing the mentioned $U_{37}^{K'}$ proxy model. However, it is important to more fully consider Prahl et al. (1988) and the possible errors stemming from its use. This is done here, as a result of developing the $U_{37}^{K'}$ proxy model.

Fig. 2 is a plot of the five data points — $U_{37}^{K'}$ from culture experiments at five different water temperatures — from the Prahl et al. (1988) culture calibration. Drawn through these points is their oft-used linear regression, i.e., Eq. 2. Additionally however, the linear extrapolation from this regression is shown, going to the maximum (1) and minimum (0) valid $U_{37}^{K'}$ and the corresponding temperatures.

A good idea of the amount and thus importance of the ocean sediment core data in these extrapolation regions, particularly the upper end, where the tropical data is, can be gotten from the coretop dataset of Müller et al. (1998), or even better, its update (148 additional coretops), Müller and Fischer (2003), which has 518 total coretops. There are 255 coretops from the tropics (24°S to 24°N), 211 with $U_{37}^{K'} > 0.86$, and 186 satisfying both conditions. Also note that in most of the papers of the described alkenone index time series database of this work, the range of validity (i.e., non-extrapolation region) of the calibration equation used is not noted.

Prahl et al. (1988) themselves suggested that there may be systematic divergence from linearity in these extrapolation regions. There has been other work on non-linear calibration regressions/extrapolations, particularly in these regions, where it can make a large difference; see for example Pelejero and Calvo (2003) and references therein. However, that work has either been for spatial calibrations, which as shown should not be used, or if for culture calibrations, not specifically for Prahl et al. (1988) (but perhaps with implications for it; e.g., Conte et al., 1998), which again is the most-used culture calibration by far in paleoclimate reconstruction, the point of this work.

Also shown in Fig. 2 then, are the quadratic, cubic and quartic regressions calculated here for Prahl et al. (1988), essentially the same as each other and clearly a better fit than the linear regression, and their corresponding extrapolations, which are clearly significantly different. $U_{37}^{K'}$ values greater than 0.87 do occur and there does not seem to be any evidence for the non-monotonic non-unique-T behavior of the quartic extrapolation so it will not be considered further. It should be emphasized again that extrapolations are inherently unknown — culture calibrations done

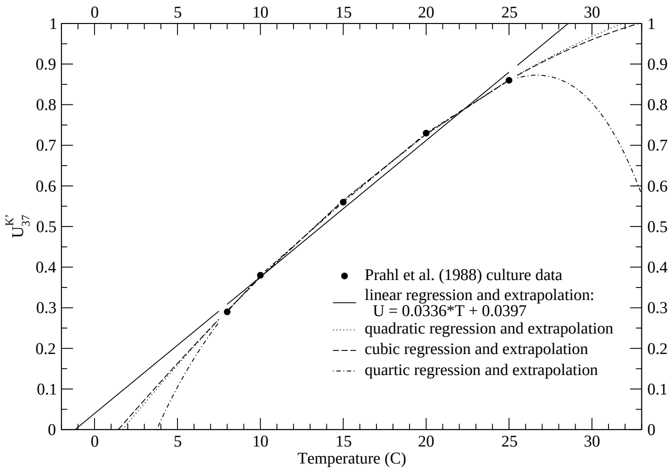

Fig. 2. $U_{37}^{K'}$ versus production (water) temperature for the culture experiments data from Prahl et al. (1988). The precision of the $U_{37}^{K'}$ measurements is given as ±0.02 for the upper three data points and ±0.03 for the next lower. Note that the linear regression was done here and so its coefficients are slightly different from those of Eq. 2 due (probably) to rounding off of values reported in Prahl et al. (1988). Also note that the quadratic, cubic, and quartic regressions are drawn but overlie each other at this scale.

in this region should be used. The extrapolation need not even be from a polynomial regression with integral powers. In the least predictable case, it could even be piecewise, i.e., non-continuous. However, among the more common regressions the cubic and similar but simpler quadratic are the extreme but still reasonable cases. The quadratic regression/extrapolation is

$$U_{37}^{K'} = -0.000550 * T^2 + 0.0516 * T - 0.0855 \quad (11)$$

Inverting so that a temperature could then be calculated from an observed $U_{37}^{K'}$ value gives (choosing the negative root in order to keep the temperature range reasonable for $U_{37}^{K'}$ between 0 and 1)

$$T = 46.93 - \sqrt{2047 - 1819 * U_{37}^{K'}} \quad (12)$$

The cubic regression/extrapolation is

$$U_{37}^{K'} = (-4.98 \times 10^{-6}) * T^3 - 0.000301 * T^2 + 0.0478 * T - 0.0677 \quad (13)$$

Solving this for T given a $U_{37}^{K'}$ value can be done in a number of ways but none are simple equations. It is probably easiest and most common to numerically solve it using iterative techniques like those based on Newton's Method, as is done in this work.

Because of the large amount of tropical data, the upper-end extrapolation region is of most interest (the lower-end extrapolation region is a problem for the same reasons but has less data and would involve the different calibration for the other alkenone index, U_{37}^{K}; see Sec. 2). To more precisely see the differences between the extrapolations, and thus the possible errors in using one instead of another, Fig. 3 is a gridded magnification of this region. Clearly, in the extrapolation region, and even in the regression region, there

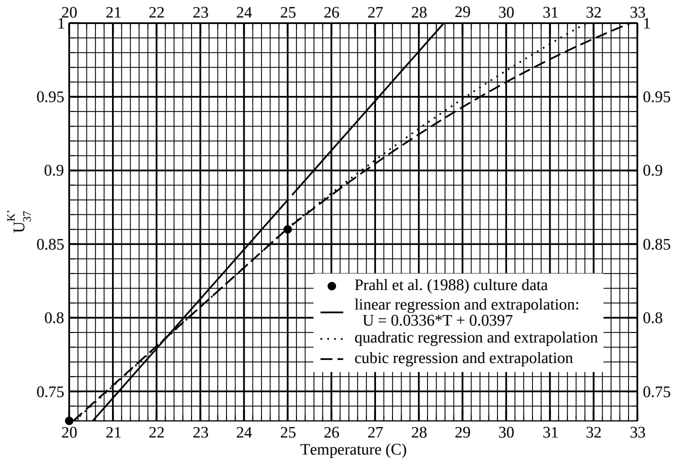

Fig. 3. Upper-end gridded magnification of Fig. 2 but with the quartic regression/extrapolation omitted.

can be significant differences, up to 4°C, between the linear regression/extrapolation and the quadratic and cubic regressions/extrapolations. Even between the quadratic and cubic extrapolations there can be significant differences, up to 1°C.

As a relevant example, the mean tropical SST from the Müller and Fischer (2003) ocean sediment coretop dataset can be calculated. However, how to calculate a "mean tropical" value from core data is problematic because cores are very unevenly geographically distributed, often (including Müller and Fischer, 2003) with many in a small area and none over large areas. Means calculated just by giving equal weight to each core will significantly bias the mean towards certain small areas. A less-biased method comes from adapting core data for use with the grids of a GCM: average the data of the cores in each grid box and then average the resulting grid box values from all boxes that have cores in them.

Moreover, the relative differences are the important point here. So, the 4° latitude by 5° longitude grid boxes (edges starting at 88°S and 180°W) of the GCM of Sec. 9 ahead are applied to the tropical coretops of Müller and Fischer (2003) (82 grid boxes, 255 coretops). Using the $U^{K'}_{37}$ measurements (with precisions of approximately ±0.01) from these coretops, the oft-used culture-based Prahl et al. (1988) inverted linear regression/extrapolation (Eq. 3) gives a mean tropical SST of 25.5°C; the Müller et al. (1998) inverted spatial calibration equation (Eq. 5), supposedly essentially the same as Prahl et al. (1988), gives 26.1°C; the never-used Prahl et al. (1988) inverted quadratic regression/extrapolation (Eq. 12) gives 27.2°C; and the never-used but more-difficult-to-calculate Prahl et al. (1988) inverted cubic regression/extrapolation gives a mean tropical SST of 27.4°C. Just calculating mean tropical SST by giving equal weight to each coretop gives: linear Prahl et al. (1988), 24.6°C; Müller et al. (1998), 25.2°C; quadratic Prahl et al. (1988), 26.1°C; and cubic Prahl et al. (1988), 26.2°C. In either case, the never-used Prahl et al. (1988) inverted non-linear regressions/extrapolations give significantly different results from the earlier ones and it is important to further note that all these averages include many cores but that most alkenone SST paleoclimate reconstructions use only a few cores, so the differences can be greater.

Calculating in the same way but using the SST over the coretops from the climatology used in Müller et al. (1998) gives a mean tropical SST of 25.9°C (just giving equal weight to each coretop gives 25.0°C). This is close to Müller et al. (1998), as expected from the origin of that inverted calibration equation. However, this may actually be another indication that Müller et al. (1998) is wrong. It is from ocean sediment coretops and while many of these are taken to be "present day" (since that is the SST used), they may actually be from sometime during the last few thousand years (i.e., late Holocene), since coretops are often not otherwise dated (e.g., Müller et al. (1998), Sec. 2.1). As indicated by many of the alkenone index time series in the database of this work, during this time tropical SST may have been warmer than the last decades going back into the pre-industrial era, which might more usually be thought of as "present day". This would be in agreement with the Prahl et al. (1988) inverted non-linear regressions/extrapolations.

A common tactic to eliminate or at least lessen biases in paleoclimate reconstructions, particularly via modelling (also in future climate prediction), is to take the difference from present day, assuming/hoping that any biases in the methods applied to both time slices will subtract out. However, this will not work with the described bias. For example, looking at Fig. 3, assume that the $U^{K'}_{37}$ value from the top of an ocean sediment core was 0.95 and the real present day SST there was 29°C, as given by the quadratic extrapolation. The linear extrapolation though, would imply 27°C. Then assume that downcore the $U^{K'}_{37}$ value was 0.78 and the real SST at that earlier time slice was 22°C, as given by the quadratic regression. The linear regression though, would also imply 22°C. Then the real temperature difference between the two time slices would be 7°C, as given by the quadratic regression/extrapolation, but the linear regression/extrapolation would imply only 5°C, which is a significant quite-possible discrepancy (remembering that the non-linear regressions/extrapolations seem to be better than the linear).

Finally, it should be noted for the upper-end extrapolation region (similarly also for the lower end) that there could be a significant effect due to measurement error when a gas chromatograph is used near its detection limit (see Grimalt et al. (2001) and references therein). This is due to preferential adsorption of $C_{37:3}$ compared to $C_{37:2}$ and results in inaccurately-high $U^{K'}_{37}$ (see Eq. 1) and thus inaccurately-high implied temperatures. However, this would not occur in all sediment core samples, only those with low C_{37} concentrations. Further, this would act as a "correction" to the described calibration extrapolation error but may disappear as this measurement error is increasingly reduced.

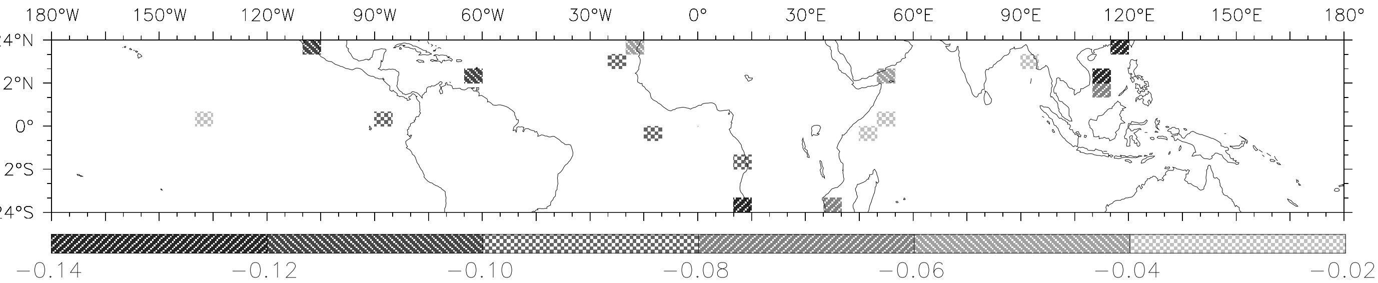

Fig. 4. Tropical map of LGM – PD $U_{37}^{K'}$ from the ocean sediment cores in each GCM grid box.

9. LGM Tropics Example

An important example of the significant errors due to the preceding that may be in many previous alkenone SST paleoclimate reconstructions and of the better method described in Sec. 7 is from the Last Glacial Maximum (LGM; 21 kyr BP) tropics.

Since CLIMAP (CLIMAP, 1981) there has been the question of whether tropical SST at the LGM were on average significantly (several degrees C) colder than present day (PD) or were not much (around a degree or less) colder. This question has implications for a basic understanding of how climate works; for example, whether the tropics are drivers of global climate. Significantly colder LGM tropical SST are indicated, although often indirectly, by most climate models and land surface air temperature proxies while nearly unchanged LGM tropical SST are indicated by the foraminiferal species assemblages method of CLIMAP. For a relevant review see Thresher (2004) (Sec. 7.2) and references therein and the earlier Broecker (2002). It was hoped more recently developed geochemical SST proxies like alkenones and foraminifera Mg/Ca would more definitively answer the question but they have also been equivocal (see for example Herbert (2003), Sec. 6.15.8.7, and references therein and Thresher (2004), Sec. 7.2.2). However, the problem, at least for alkenones, may have been as shown in this work. For example, MARGO (Multiproxy Approach for the Reconstruction of the Glacial Ocean surface; Kucera et al. (2005) and references therein) was a recent project applied to CLIMAP SST results and its alkenone SST data, gathered in Rosell-Melé et al. (2004), was originally from other paleoclimate reconstructions, done as usual using either the linear Prahl et al. (1988) or Müller et al. (1998) calibrations (noted again in Rosell-Melé et al. (2004) to be much the same).

9.1. *Errors From Calibration Extrapolations*

To see the significant errors possible in previous alkenone SST paleoclimate reconstructions, the method of the PD tropics example in Sec. 8 can be applied to the described ocean sediment core alkenone time series database of this work for the LGM and PD time slices and then the LGM minus PD difference (LGM – PD) looked at. The LGM time slice $U_{37}^{K'}$ is the average of all downcore measurements between 22.5 and 19.5 kyr BP (i.e., 21 ± 1.5 kyr BP) and the PD time slice is between 3 and 0 kyr BP. LGM – PD is used instead of just LGM in order to eliminate/lessen any biases, although not the one discussed in Sec. 8, and to be consistent with the paleoclimate modelling to be discussed. There are 17 tropical grid boxes containing 19 cores (see Appendix 2), many of which were in Rosell-Melé et al. (2004). Some tropical grid boxes, and so tropical cores in the database, are not used because there are not cores in them with both LGM and PD values or because they are outside the LGM ocean mask of the GCM grid in the paleoclimate simulations to be discussed (due to sea level being lower at the LGM than at PD there are more land grid boxes in the LGM climate simulation). Fig. 4 is a tropical map of LGM – PD $U_{37}^{K'}$ from the cores. Note the sometimes large differences between nearby grid boxes and that the precision of the $U_{37}^{K'}$ measurements is given as ±0.01 for most cores, as good as ±0.005 for a few cores, and no worse than ±0.017 for just a couple of cores.

Concentrating on the relative differences between them then (i.e., the possible errors in using one instead of another), the oft-used culture-based Prahl et al. (1988) inverted linear regression/extrapolation (Eq. 3) gives an LGM – PD mean tropical SST of -2.2°C; the Müller et al. (1998) inverted spatial calibration equation (Eq. 5), supposedly essentially the same as Prahl et al. (1988), gives -2.3°C; using whatever inverted calibration equation is in each core's publication (Prahl et al. (1988) or Müller et al. (1998) usually) gives -2.3°C; the never-used Prahl et al. (1988) inverted quadratic regression/extrapolation (Eq. 12) gives -3.1°C; and the never-used Prahl et al. (1988) inverted cubic regression/extrapolation gives an LGM – PD mean tropical SST of -3.3°C. The never-used Prahl et al. (1988) inverted non-linear regressions/extrapolations give significantly larger magnitude results than the linear Prahl et al. (1988) or Müller et al. (1998) usually used in paleoclimate reconstructions, including those applied to the CLIMAP-instigated LGM – PD tropical SST controversy. Finally, it is worth noting again that all these averages include relatively many cores but that most alkenone SST paleoclimate reconstructions use only a few cores, so the differences can be greater.

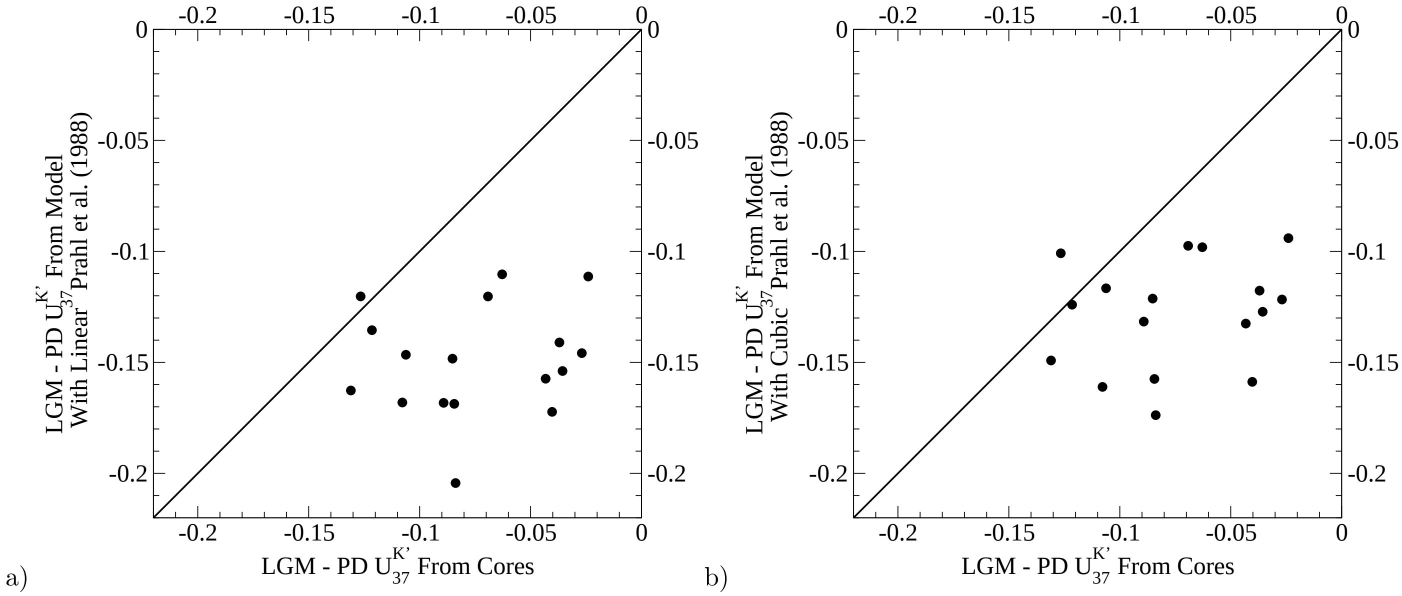

Fig. 5. For tropical grid boxes, LGM − PD $U_{37}^{K'}$ from the models versus the cores for the $U_{37}^{K'}$ proxy models using: a) the Prahl et al. (1988) linear calibration equation; and b) the Prahl et al. (1988) cubic calibration equation. Not shown are the results from the $U_{37}^{K'}$ proxy models using the Müller et al. (1998) calibration equation and the Prahl et al. (1988) quadratic calibration equation because they are nearly indistinguishable at this scale from a and b, respectively. Perfect matches between models and cores would be on the 1:1 diagonal line (it is not a linear regression). The precision of the $U_{37}^{K'}$ measurements is given as ±0.01 for most cores, as good as ±0.005 for a few cores, and no worse than ±0.017 for just a couple of cores.

9.2. *Better Paleoclimate Reconstruction Method*

The better alkenone temperature paleoclimate reconstruction method compares directly to the ocean sediment core $U_{37}^{K'}$, justifiably treating it as a much less questionable reference. The best possible climate simulations are done with the most sophisticated climate models and the results are input into a proxy model of how $U_{37}^{K'}$ is affected by climate. Here those climate simulations are of the LGM and PD using a full coupled atmosphere-ocean GCM (AOGCM), which predict SST (as well as temperatures at all other depths) for input to the proxy model; see Appendix 3 for further description but note in the following that the mean annual results are used except where stated otherwise. However here, the incipient $U_{37}^{K'}$ proxy model is just one of the discussed calibration equations, uninverted, and all are tested, which is one of the advantages of this method. Note that Rosell-Melé et al. (2004) also does comparisons to GCM simulations with its alkenone data but it compares GCM SST to SST from the usual application of the linear Prahl et al. (1988) or Müller et al. (1998) calibrations, which as shown in this work is distinctly different and not a good method. Note also that Giraud (2006) is work on a $U_{37}^{K'}$ proxy model but, while more advanced (perhaps overly) in many ways than the incipient model here, uses the spatial calibration of Müller et al. (1998) and is built into only a regional ocean model (applied partially in the tropics).

Using the Prahl et al. (1988) linear calibration equation (Eq. 2) in the $U_{37}^{K'}$ proxy model here gives an LGM − PD mean tropical $U_{37}^{K'}$ of -0.1491; using the Müller et al. (1998) calibration equation (Eq. 4) gives -0.1447; using the Prahl et al. (1988) quadratic calibration equation (Eq. 11) gives -0.1282; and using the Prahl et al. (1988) cubic calibration equation (Eq. 13) in the $U_{37}^{K'}$ proxy model gives an LGM − PD mean tropical $U_{37}^{K'}$ of -0.1284. The LGM − PD mean tropical $U_{37}^{K'}$ from the cores is -0.0750. All averaging is by GCM grid box as described. The Prahl et al. (1988) non-linear calibrations clearly improve the match between the model and the cores (the slightly better match of the Prahl et al. (1988) quadratic calibration equation compared to the cubic, when the opposite might be expected, may be from accumulated numerical error after iterated non-linear calculations).

Single averages can be misleading so Fig. 5 is plots for tropical grid boxes of LGM − PD $U_{37}^{K'}$ from the models versus the cores, which are the independent reference. Only the plots for the $U_{37}^{K'}$ proxy models using the Prahl et al. (1988) linear calibration equation and the Prahl et al. (1988) cubic calibration equation are shown because the results from that using the Müller et al. (1998) calibration equation are nearly indistinguishable at this scale from the former and the results from that using the Prahl et al. (1988) quadratic calibration equation are nearly indistinguishable from the latter. In each plot, perfect matches between model and cores would be on the 1:1 diagonal line (it is not a linear regression). Since most of its points are clearly closer to this line (in the vertical direction since the cores are the reference), the $U_{37}^{K'}$ proxy model using the Prahl et al. (1988) cubic calibration equation is significantly better than that using the Prahl et al. (1988) linear calibration equation (and thus the Müller et al. (1998) calibration equation). This is

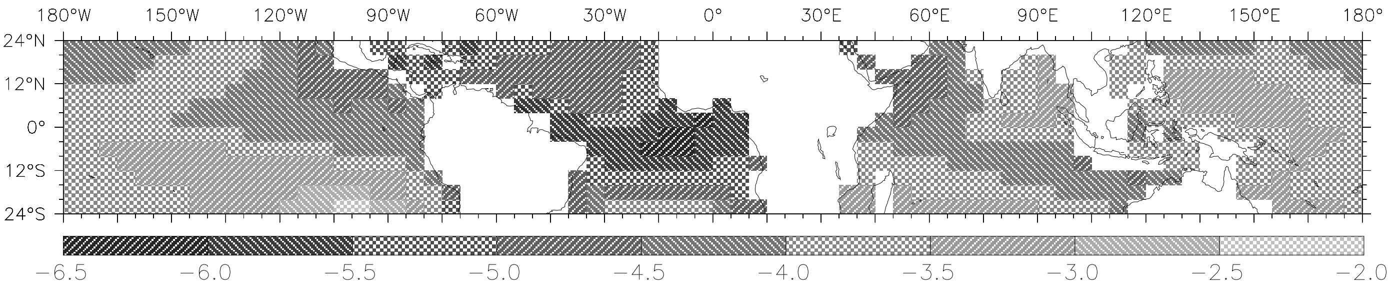

Fig. 6. Tropical map of LGM − PD mean annual SST (C) from AOGCM climate simulations. Note that this is the LGM land mask with PD real-world land outlines drawn in and it more than encompasses all land grid boxes from the PD time slice (see Sec. 9.1).

not absolute proof, since the climate simulations could be biased (even doing LGM − PD), but it is a good indication.

The distribution of the points in Fig. 5b still might not be considered impressive but this may just indicate the need for a better proxy model than simply here the calibration equation of the incipient $U_{37}^{K'}$ proxy model using GCM SST, i.e., a proxy model that accounts for more of the complicating factors of Sec. 3.

Furthermore, as indicated by both the averages and Fig. 5b, there does still seem to be a mean bias in the model compared to the cores. The reason for this may be that PD is defined, particularly via greenhouse gas concentrations, as around 1978 A.D. for the climate simulations (see Appendix 3) and not as pre-industrial, which the given definition of PD for the cores could be more appropriate for. Due to global warming the PD climate simulations here would tend to be warmer than pre-industrial ones and make the LGM − PD mean tropical $U_{37}^{K'}$ more negative (warmer PD SST, larger PD $U_{37}^{K'}$, more negative LGM − PD $U_{37}^{K'}$). Estimating up to a degree C warming in mean tropical SST from the pre-industrial era to PD and looking at the temperatures the model minus core mean tropical $U_{37}^{K'}$ differences (≈ 0.5) imply in Fig. 3, this could explain a large part of the mean bias and suggest that the cores agree better with the climate simulations.

As indicated, the specific month alkenones are from is unknown. Using the climate simulation results from February or August — the annual extremes and the only months CLIMAP was done for — instead of the mean annual results does not significantly change any of the preceding analysis, although August seems to give just slightly better matches to the cores.

Finally then, since the main goal is to reconstruct paleoclimate, from the AOGCM climate simulations, using only the grid boxes with cores, the LGM − PD mean tropical annual SST is -4.4°C. A big advantage of climate models over just ocean sediment cores is that they can indicate SST over the entire tropics and allow calculating a real all-tropic mean. So using all tropical grid boxes (ocean boxes common to both LGM and PD time slices; see Sec. 9.1) the LGM − PD mean tropical annual SST is -4.1°C. For a pre-industrial time slice instead of PD as defined here, this might be up to a degree C more positive, as discussed. Fig. 6 is a tropical map of LGM − PD mean annual SST from the AOGCM climate simulations. Note the significant spatial variation, which may make means misleading at any individual site.

10. Conclusion

Inversions of spatial $U_{37}^{K'}$(SST) calibration equations should not be used as paleoSST equations. It might be argued that this is not currently a problem since the most popular one, Müller et al. (1998), is so similar to the most popular inverted culture $U_{37}^{K'}$(T) calibration equation, Prahl et al. (1988). However, culture calibrations by themselves, the usual method, make no attempt to account for climate and other factors, as they would when used with the better method described in this work. Further, the linear regression of Prahl et al. (1988) is used and often, such as in the tropics where there is much alkenone data, it is used outside its valid range, where its never-used non-linear extrapolations are probably significantly better.

A better method to use the alkenone index as a temperature proxy and reconstruct paleoclimate is to do the best possible paleosimulations with the most sophisticated global climate models to physically-consistently take care of the climate factors, input the results to a proxy model of how the alkenone index is affected by climate and other factors and then directly validate the results with a large global database of alkenone index paleorecords. It is important to use the alkenone data in the best manner possible to reconstruct paleoclimate because it is probably one of the better climate proxies (relatively straightforward and well-preserved) and is expensive, difficult, and time-consuming to put together — it should not be misinterpreted in the last step to reconstructing paleoclimate.

With this better method, culture calibration work, which is also expensive, difficult, and time-consuming, is fundamental and critical and more such work should be done, and more done with the results. Furthermore, ocean sediment core alkenone data should be reported as the raw alkenone index values, not just as SST values from using an inverted calibration equation; among 77 cores in the alkenone time series database, 30 were reported without the raw alkenone index values (see Appendix 1).

Using this better method, non-linear regressions/extrapolations of the culture $U_{37}^{K'}$(T) calibration of Prahl et al.

(1988) seem better than the usual linear regressions/extrapolations of it or the spatial $U_{37}^{K'}(T)$ calibration of Müller et al. (1998). And then alkenones seem to be consistent with climate models on the CLIMAP-instigated LGM – PD tropical SST controversy and confirm a significant LGM – PD tropical SST difference.

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Table A1
Tropical ocean sediment cores used in this work.

Core	Latitude	Longitude	Reference(s)
GeoB1710-3	23° 25.8′ S	11° 42′ E	Kirst et al. (1999)
MD79257	20° 24′ S	36° 20′ E	Bard et al. (1997), Sonzogni et al. (1998)
ODP1078C	11° 55.24′ S	13° 24.01′ E	Kim et al. (2003)
GeoB1016-3	11° 46.2′ S	11° 40.9′ E	Schneider et al. (1995)
GeoB1105-3	1° 39.9′ S	12° 25.7′ W	Müller et al. (1998)
GeoB1105-4	1° 39.9′ S	12° 25.7′ W	Schneider et al. (1996)
MD85668	0° 1′ S	46° 2′ E	Bard et al. (1997)
Y69-71P	0° 4.98′ N	86° 28.92′ W	Prahl et al. (2006)
W8402A-14GC	0° 57.2′ N	138° 57.3′ W	Prahl et al. (1989), Jasper et al. (1994)
MD85674	3° 11′ N	50° 26′ E	Bard et al. (1997)
17961	8° 30.4′ N	112° 19.9′ E	Pelejero et al. (1999), Wang et al. (1999)
M35003-4	12° 5′ N	61° 15′ W	Rühlemann et al. (1999)
TY93-929/P	13° 42′ N	53° 15′ E	Rostek et al. (1997)
17954	14° 47.8′ N	111° 31.5′ E	Pelejero et al. (1999), Wang et al. (1999)
BOFS31K	19° 0′ N	20° 10′ W	Chapman et al. (1996)
SO93-126KL	19° 58.4′ N	90° 2.03′ E	Kudrass et al. (2001)
17940	20° 7.0′ N	117° 23.0′ E	Pelejero et al. (1999) Wang et al. (1999)
ODP658C	20° 45′ N	18° 35′ W	Zhao et al. (1995), deMenocal et al. (2000)
LPAZ21P	22° 59.4′ N	109° 28′ W	Herbert et al. (2001)

Appendix 1. Ocean Sediment Core Alkenone Time Series Database

Starting in Thresher (2004) an up-to-date database of ocean sediment core alkenone time series has been carefully compiled. As of October 2006 it contained data for 77 cores. Since there are documentation problems even with core data that have publications describing it, no core data without such publications is included. Some core data with such publications is not made available by the authors so is not included. Another inclusion criterion is the ocean sediment core age model. Since there are known significant errors, no core data using only uncalibrated ^{14}C dates as the age model is included. Most age models are SPECMAP-based or use calibrated ^{14}C dates, with ocean reservoir age corrections, if any, as given by the authors; the remaining few types of included age models are also based on calendar dates, e.g., comparison to ice cores. The authors themselves are a major source for the core data, followed by the PANGAEA environmental database and the NOAA data centers. To be used as in this work, a considerable amount of processing is necessary even after obtaining the core data. During this and considerably-often, discrepancies in the original data are noted and these are attempted to be fixed in collaboration with the authors; if serious (e.g., age paradoxes) and unresolved, the core data is not included. Much of the core data as provided does not give the raw $U_{37}^{K'}$ values so these are calculated using the given SST values and the $U_{37}^{K'}$(SST) calibration equation indicated in the core's publication.

Appendix 2. Tropical Ocean Sediment Cores Used

See Table A1.

Appendix 3. Climate Model and Simulations

A version of the GISS non-flux-adjusted coupled atmosphere (Hansen et al., 2002) / ocean (Russell et al., 1995) primitive-equation GCM was used. It has a resolution of 4° latitude by 5° longitude, with 9 hybrid terrain-following/pressure levels in the atmosphere and up to 13 increasingly-thick bathymetry-dependent levels in the ocean. It includes a thermodynamic/dynamic sea ice model, a sub-grid-scale straits parameterization, and a land surface model that can account for glaciers, variously-vegetated ground, and lakes, including specified runoff/river directions. Era-appropriate boundary conditions were set based on recent research: sea-level/isostasy-dependent topography (Peltier and Solheim, 2001), continental glaciers (Peltier and Solheim, 2001), straits, mean ocean salinity (based on ocean volume from Peltier and Solheim (2001) and constant total salt), insolation (Berger, 1978), and greenhouse gas concentrations. Aerosols, vegetation and iceberg calving, all little-known for past eras, were left as for present day (PD), with minor exceptions. PD is defined, primarily by the insolation and greenhouse gases, as 1978 A.D. For a more complete description see Thresher (2004).

Using only parallel computing for acceleration, the LGM and PD simulations were run for 1120 and 880 model years, respectively, and their last 100 years averaged. During the averaging century for the LGM simulation the global mean temperature and salinity of the deepest possible ocean layer changed by −0.05°C and 0.010 g/kg, respectively; for the PD simulation, by 0.03°C and 0.008 g/kg. It is thus considered to be sufficiently near equilibrium. Thresher (2004) applies only for results after about the first half of the model years run.